$$\frac{\partial u_i}{\partial t} + u_j \frac{\partial u_i}{\partial x_j} = -\frac{1}{\rho}\frac{\partial p}{\partial x_i} + \nu \frac{\partial^2 u_i}{\partial x_j^2}$$

$\nu = \frac{\mu}{\rho}$

$\frac{\partial^2}{\partial x_j \partial x_j}$

Tutorial

Intro to probability theory

① Sample space & probability

(1.1) $\Omega = \{$"All possible outcomes of an experiment"$\}$

Example

E1) ~~Roll~~ Roll a Dice $\Omega = \{1,2,3,4,5,6\}$

E2) Flip a coin $\Omega = \{'H','T'\}$

E3) Roulette $\Omega = \{1,2,\dots\} \cong \mathbb{N}$ ∈ How many times until we get red?

For now: Finite or countably infinite sample space

(1.2) Events $A \subseteq \Omega$

Example: (E1) 'Even no.' $A = \{2,4,6\} \subset \Omega$

Elementary event: Singleton set containing 1 element $\omega \in \Omega$

$A = \{\omega\}$

(1.3) Probability: $P: \mathcal{P}(\Omega) \to [0,1]$ s.t $P(\Omega) = 1$

↑ Power set

finite Ω: $P(A_1) + P(A_2) = P(A_1 \cup A_2)$ $A_1 \cap A_2 = \emptyset$

infinite Ω: $\sum_{n=1}^{\infty} P(A_n) = P\left(\bigcup_{n=1}^{\infty} A_n\right)$

We call (Ω, P) a probability space

Ex (E1) Even no. A_1, odd no. A_2

$= \{2,4,6\} \subset \Omega$ $= \{1,3,5\}$

If we assume $P(\{\omega_i\}) = 1/6$ $i = 1:6$

$P(A_1) = \frac{1}{2} = P(A_2)$

$P(A_1 \cup A_2) = P(A_1) + P(A_2) = 1$

Probability function $P(\{\omega_i\}) = p(\omega_i)$ ⇒ $1 = \sum_{\omega \in \Omega} p(\omega)$ 'prob. of elementary event'

Laplace model → $p(\omega) = \frac{1}{\#\Omega}$ $P(A) = \frac{\#A}{\#\Omega}$

E3 $P(1) = \frac{18}{37}$ getting red on 1st try

$P(2) = \frac{19}{37} \cdot \frac{18}{37}$

$P(3) = \left(\frac{19}{37}\right)^2 \frac{18}{37}$

$P(n) = \left(\frac{19}{37}\right)^{n-1} \frac{18}{37}$ $\quad \sum_{n=1}^{\infty} P(n) = 1$

(1.4) Multivariate probability

$\Omega^n = \Omega \times \Omega \cdots \times \Omega = \{(a_1, \ldots a_n) : a_i \in \Omega\}$

Example 'Two dice' $\Omega^2 = \Omega \times \Omega \xleftarrow{E1} = \{(a_1, a_2) : a_i \in \Omega\}$

$\omega_i \in \Omega^2 = (a_1, a_2)$ $\quad P(\omega_i) = 1/36$

(2) Random variables

$X : \Omega \to R$

$P(X = a) = P(a) = \sum_{\substack{\omega \in \Omega \\ X(\omega) = a}} P(\omega)$

E4 Ed Two dice' $\omega = (i, j)$ $\quad i, j = 1 : 6$

$X(\omega) = i + j$

$\{\omega \in \Omega : X(\omega) = 5\} = (X = 5) = \{(1,4)(4,1)(3,2)(2,3)\}$

$P(X = 5) = \frac{1}{9}$

E2 $\{H, T\}$ $\quad X(\text{heads}) = 1$

$X(\text{tails}) = -1$

(E1) 1 die ⊛ $X(\omega) = \begin{cases} -2000 & \omega = \{1,2,3,4\} \\ 5000 & \omega = \{5,6\} \end{cases}$

(3) Moments

(3.1) Expectation value $\mu(X) = \sum_{\omega \in \Omega} X(\omega) P(\omega)$

⊛ $\mu(X) = -2000 \cdot \frac{2}{3} + 5000 \cdot \frac{1}{3} = \frac{1000}{3}$

(3.2) $\mu(F(X)) = \sum_{\omega \in \Omega} F(X(\omega)) P(\omega)$

eg. $\mu_a(X^k) = \sum_{\omega \in \Omega} X^k P(\omega)$

E2 $P(1) = \frac{18}{37}$ getting red at 1st try

$P(2) = \frac{19}{37} \cdot \frac{18}{37}$

$P(3) = \left(\frac{19}{37}\right)^2 \frac{18}{37}$

$P(n) = \left(\frac{19}{37}\right)^{n-1} \frac{18}{37}$ $\quad \sum_{n=1}^{\infty} P(n) = 1$

(1.4) Multivariate probability

$\Omega^n = \Omega \times \Omega \times \cdots \times \Omega = \{(a_1, \ldots, a_n) : a_i \in \Omega\}$

Example 'Two dice' $\Omega^2 = \Omega \times \Omega \leftarrow E1 = \{(a_1, a_2) : a_i \in \Omega\}$

$\omega_i \in \Omega^2 = (a_1, a_2)$ $\quad P(\omega_i) = 1/36$

(2) Random variables

$X : \Omega \to R$

$P(X=a) = P(a) = \sum_{\substack{\omega \in \Omega \\ X(\omega)=a}} P(\omega)$

Eg E1 'Two dice' $\omega = (i, j)$ $\quad i, j = 1:6$

$X(\omega) = i + j$

$\{\omega \in \Omega : X(\omega) = 5\} = (X = 5) = \{(4,1)(3,2)(2,3)\}$

$P(X=5) = \frac{1}{9}$

E2 $\{H, T\}$ $\quad X(\text{heads}) = 1$, $X(\text{tails}) = -1$

(E1) 1 die (*) $X(\omega) = \begin{cases} -2000 & \omega = \{1,2,3,4\} \\ 5000 & \omega = \{5,6\} \end{cases}$

(3) Moments

(3.1) Expectation value $\mu(X) = \sum_{\omega \in \Omega} X(\omega) P(\omega)$

(*) $\mu(X) = -2000 \cdot \frac{2}{3} + 5000 \cdot \frac{1}{3} = \frac{1000}{3}$

(3.2) $\mu(F(x)) = \sum_{\omega \in \Omega} F(X(\omega)) P(\omega)$

eg. $\mu_a(X^k) = \sum_{\omega \in \Omega} X^k P(\omega)$

$$\left(\underline{c}'\right) = F(c.z) = \left(F_1(c.z) \mid (*)\right.$$

Example

Variance $\sigma^2(X) = \mu((X-\mu(X))^2)$

$$= \mu\left(X^2 - 2X\mu(X) + \mu(X)^2\right)$$

$$= \mu(X^2) - 2\mu(X)^2 + \mu(X)^2$$

$$= \mu(X^2) - \mu(X)^2$$

(3.3) Standardized distribution

$$X \to X^* = \frac{X - \mu(X)}{\sigma(X)} \Rightarrow \mu(X^*) = 0$$

$$\sigma(X^*) = 1$$

(4) Information Entropy

(4.1) 'Self information' or 'surprise'

$$I(\omega) = -\log_b p(\omega) \geq 0$$

Example

$p(\omega) = 1 \Rightarrow I(\omega) = 0$

$p(\omega) \to 0 \Rightarrow I(\omega) \to \infty$

$b = 2$ (E2) $\Omega = \{'H', 'T'\}$

$p(\omega) = 1/2$

$\Rightarrow I(\omega) = 1$

(4.2) Information Entropy $H = \mu(I) = -\sum_{\omega \in \Omega} p(\omega) \log_b(p(\omega))$

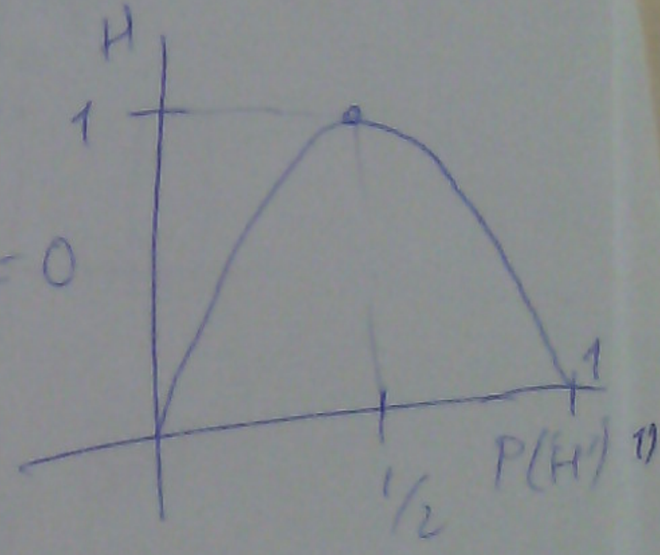
(E2) $\Omega = \{'H', 'T'\}$

(i) 'fair coin' $p(\omega) = 1/2$

$H = 1$

(ii) 'bias coin' $P(H) = 1$ $P(T) = 0$

$H = 0$



(5) Continuous Sample space

(5.1) Probability density function.

$f: \mathbb{R} \to [0, \infty)$

$\int_{\mathbb{R}} f \, dx = 1$

$P(a \leq x \leq b) = \int_a^b f \, dx$

Example: Gaussian distribution

$$f(x) = \frac{1}{\sqrt{2\pi}\sigma} e^{\frac{-(x-\mu)^2}{2\sigma^2}} = N(\mu, \sigma)$$

multivariate case

$$f: R^n \to [0, \infty)$$

$$x = (x_1, \dots x_n)$$

$$\int_{R^n} f \, dx_1 \dots dx_n = 1$$

(5.2) Moments

$$\mu(x) = \int_R x f(x) dx$$

multivariate case

$$\mu(x_k) = \int_{R^n} x_k f(x) \frac{dx_1 \dots dx_n}{d\underline{x}}$$

(5.3) Entropy

$$H(f) = -\int_{R^n} f \ln(f) d\underline{x}$$

(6) Central limit theorem

Consider E2 $\Omega = \{'H', 'T'\}$

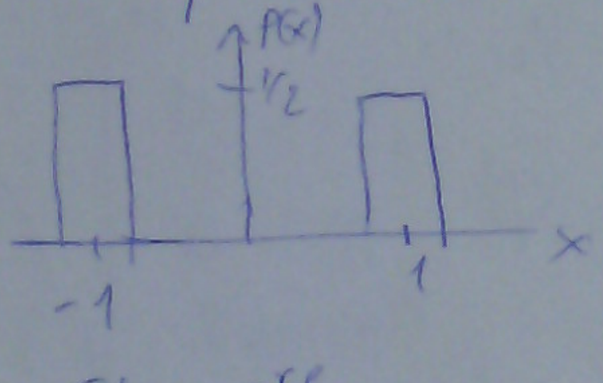
$P(\omega) = 1/2 \quad \omega \in \Omega$

$X('H') = -1$

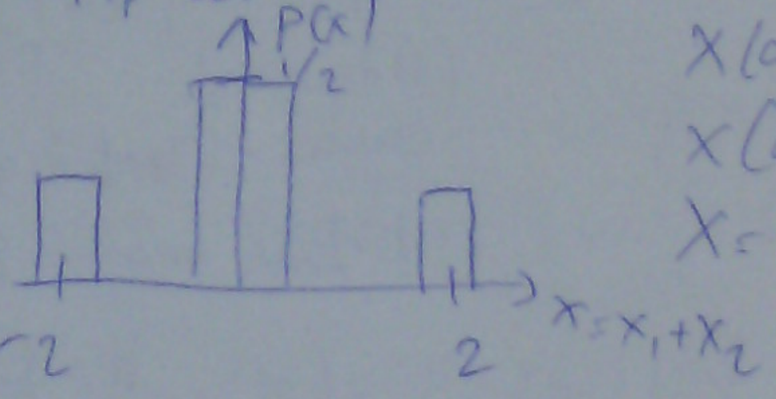
$X('T') = 1$

$\mu(X) = 0$

Flip coin once



Flip coin twice



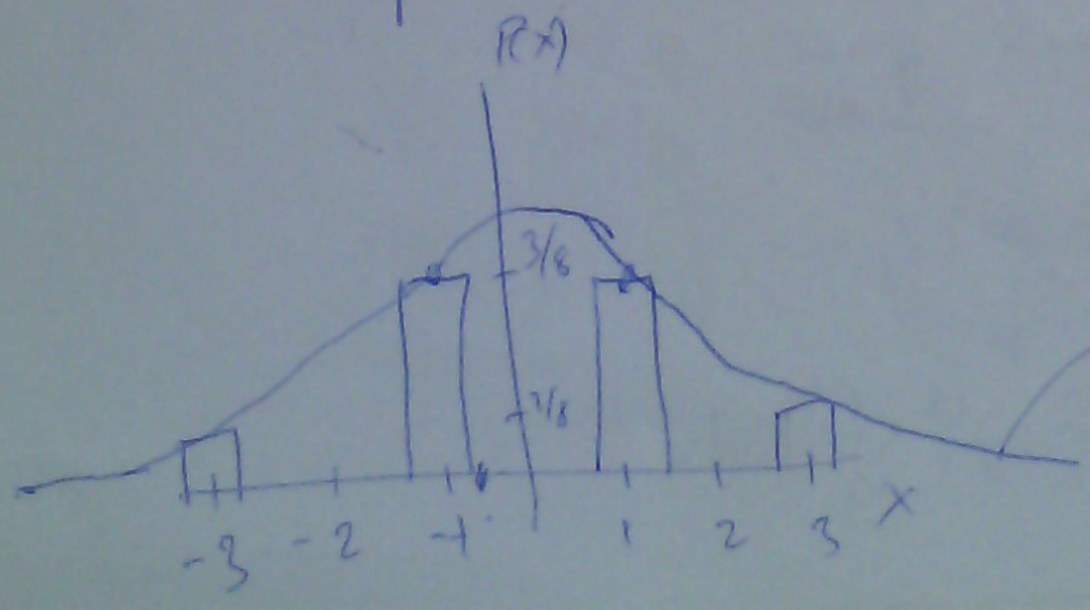
$\Omega^2 = \Omega \times \Omega$

$X(a_1) = X_1$

$X(a_2) = X_2$

$X = X_1 + X_2$

Flip 3



$$\left(\frac{c'}{n}\right) = F(c \geq z) - \left[F_1(c \geq z)\right] \quad \square$$

Theorem: Let $X_1 - - - X_n$ be independent, identically distributed (iid) random variables

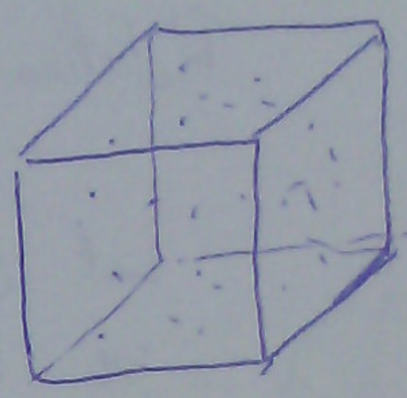
$$a_n = S_n = X_1 + - - - X_n$$

$$\lim_{n\to\infty}\left(\frac{S_n - \mu(S_n)}{\sigma(S_n)}\right) = N(0,1) = \frac{1}{\sqrt{2\pi}} e^{-\frac{x^2}{2}}$$

28/10 (4) Maxwell - Boltzmann Distribution

$\rho = \rho_0$, $T = T_0$ } constant.

neglect external forces

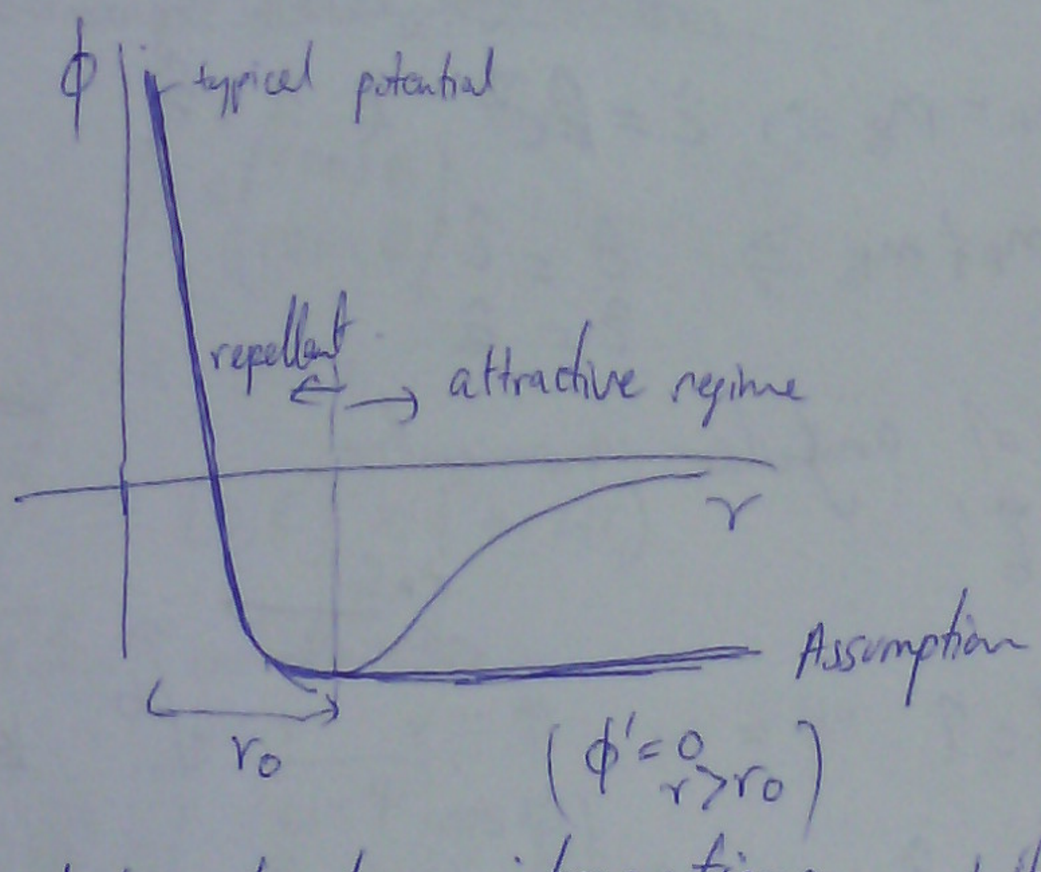


Gas in a box

Intermolecular forces?

Assume - binary interactions
- spherically symmetric potentials

force $F = -\phi'(r)$



4.1 Intermolecular interactions

Consider two particles m_A, $\underline{c}$ (velocity) & m_B, $\underline{z}$

at $t=0$ $\underline{X}_A$ (position) $\underline{X}_B$ 1)

$$\underline{X}_m = \frac{X_A m_A + X_B m_B}{m_A + m_B}$$

$$\underline{W} = \dot{\underline{X}}_m = \frac{\dot{X}_A m_A + \dot{X}_B m_B}{m_A + m_B} = \frac{\underline{c}(t) m_A + \underline{z}(t) m_B}{m_A + m_B}$$

$\underline{W}$ constant velocity

$$F' = \begin{pmatrix} \frac{\partial F_1}{\partial \underline{c}} & \frac{\partial F_1}{\partial \underline{z}} \\ \frac{\partial F_2}{\partial \underline{c}} & \frac{\partial F_2}{\partial \underline{z}} \end{pmatrix}$$ 3×3 matrices

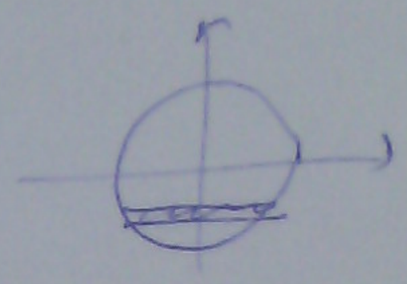
$$\det F' = 1$$

3/11

① Integral Transformation

Motivation:

Let $D = \{(x,y) : x^2+y^2 \leq R^2 ; R>0\}$



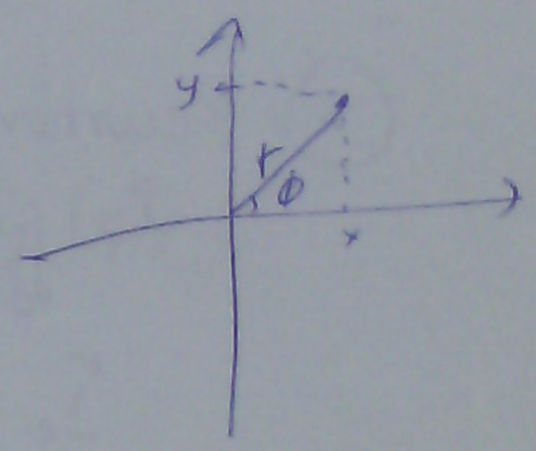
Consider

$$\iint_D f(x,y)\,dx\,dy = \int_{-R}^{R} \int_{-\sqrt{R^2-y^2}}^{+\sqrt{R^2-y^2}} f(x,y)\,dx\,dy$$

Let $\Phi : S \to D$ be coordinate transformation

$$(u,v) \to \Phi(u,v) = (x,y)$$
$$(u,v,w) \to \Phi(u,v,w) = (x,y,z)$$

Example a) Polar coordinates $u = r$, $v = \phi$

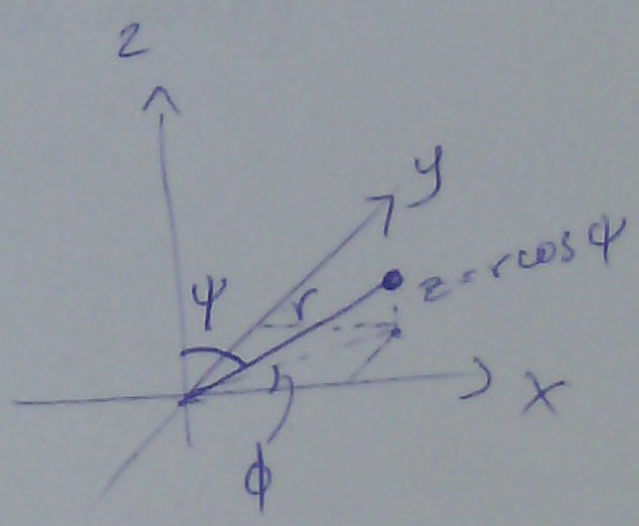


$$\Phi = \begin{pmatrix} r\cos\phi \\ r\sin\phi \end{pmatrix}$$

D is same

$$S = [0,R] \times [0,2\pi)$$

b) Polar coordinates $u = r$ $v = \phi$ $w = \psi$



$$\Phi(r,\psi,\phi) = \begin{pmatrix} r\sin\psi\cos\phi \\ r\sin\psi\sin\phi \\ r\cos\psi \end{pmatrix}$$

$$D = \{(x,y,z) : x^2+y^2+z^2 \leq R^2\}$$

$$S = [0,R] \times [0,\pi] \times (0,2\pi)$$

$$\int_D dx\,dy\,dz = \int_S |\det \Phi'|\,du\,dv\,dw$$

magnitude of vector

so $(0,\pi/2)$ due to symmetry

Example

a) $\underline{\phi}(r,\phi) = \begin{pmatrix} r\cos\phi \\ r\sin\phi \end{pmatrix}$

$$\underline{\phi}'(r,\phi) = \begin{pmatrix} \cos\phi & -r\sin\phi \\ \sin\phi & r\cos\phi \end{pmatrix}$$

$$\det(\underline{\phi}') = r$$

$$\int_D dx\,dy = \int_0^{2\pi}\int_0^R r\,dr\,d\phi$$

b) $$\underline{\phi}(r,\psi,\phi) = \begin{pmatrix} r\sin\psi\cos\phi \\ r\sin\psi\sin\phi \\ r\cos\psi \end{pmatrix}$$

$$\phi'(r,\psi,\phi) = \begin{pmatrix} \sin\psi\cos\phi & r\cos\psi\cos\phi & -r\sin\psi\sin\phi \\ \sin\psi\sin\phi & r\cos\psi\sin\phi & r\cos\psi\cos\phi \\ \cos\psi & -r\sin\psi & 0 \end{pmatrix}$$

$$\det(\phi') = r^2\cos^2\psi\cos\phi + r^2\sin^2\psi\sin^2\phi + r\cos^2\psi\sin\psi\sin^2\phi$$

$$= r^2\sin\psi$$

$$\int_D dx\,dy\,dz = \int_S r^2\sin\psi\,dr\,d\psi\,d\phi$$

(2) Recursion formulae

for $\int_0^\infty x^n e^{-ax^2}dx = \underline{I}_n$

$$\underline{I}_0 = \int_0^\infty e^{-ax^2}dx$$

$$\underline{I}_0^2 = \int_0^\infty e^{-ax^2}dx\int_0^\infty e^{-ay^2}dy = \int_0^\infty\int_0^\infty e^{-a(x^2+y^2)}dx\,dy$$

$$= \int_0^{\pi/2}\int_0^\infty e^{-ar^2} r\,dr\,d\phi$$

$$= \frac{\pi}{2}\int_0^\infty e^{-ar^2} r\,dr \qquad z = ar^2$$

$$= \frac{\pi}{4a}\left(-e^{-z}\right)_0^\infty$$

$$\underline{I}_0 = \sqrt{\frac{\pi}{4a}} = \frac{1}{2}\sqrt{\frac{\pi}{a}}$$

(ii) $\underline{I}_1 = \int_0^\infty x\,e^{-ax^2}dx = 1/2a$

(iii) $$\frac{d}{da}\underline{I}_n = \frac{d}{da}\int_0^\infty x^n e^{-ax^2}dx$$

$$= \int_0^\infty x^n \frac{d}{da} e^{-ax^2} dx = \int_0^\infty x^{n+2} e^{-ax^2} dx$$

$$\frac{d}{da}(I_n) = -I_{n+2}$$

$$I_n = -\frac{d}{da} I_{n-2} \qquad n = 2, 3 \ldots$$

$$I_2 = \frac{1}{4}\sqrt{\frac{\pi}{a^3}}$$

$$I_4 = \frac{3}{8}\sqrt{\frac{\pi}{a^5}}$$

Remark $\tilde{I}_n = \int_{-\infty}^{\infty} x^n e^{-ax^2} dx$

$\tilde{I}_n = 0$ n odd

$\tilde{I}_n = 2I_n$ n even

(3) Gaussian / Maxwell distribution

Let $\hat{f}(\underline{c})$ be pdf

normalize $f(\underline{c}) = n\hat{f}(\underline{c})$

↳ number density $[n] = m^{-3}$

Note

$$n = \int_{\mathbb{R}^3} f(\underline{c}) d\underline{c}$$

we define $\underline{u} = \frac{1}{n}\int_{\mathbb{R}^3} \underline{c} f(\underline{c}) d\underline{c}$ 'bulk velocity'

$$\frac{3}{2} k_B T = \frac{1}{n}\int_{\mathbb{R}^3} \frac{m}{2} \underbrace{|(\underline{u} - \underline{c})|^2}_{\xi} f(\underline{c}) d\underline{c}$$

$\xi \rightarrow$ thermal velocities

Tomorrow: In equilibrium

$$f(\underline{c}) = A e^{-B^2 |\underline{c} - \underline{\alpha}|^2}$$

Consider

$$n = \int_{\mathbb{R}^3} f(\underline{c}) d\underline{c} \overset{\xi = c - \alpha}{=} \int_{\mathbb{R}^3} f(\xi) d\xi$$

$$= A \int_{\mathbb{R}^3} e^{-\beta(\xi_1^2 + \xi_2^2 + \xi_3^2)} d\xi_1 d\xi_2 d\xi_3$$

$$= A \left(\int_{\mathbb{R}^1} e^{-\beta^2 \xi^2} d\xi\right)^3$$

$$= \frac{A\pi^{3/2}}{|B|^3}$$

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$$n = \frac{A\,\pi^{3/2}}{|\beta|^3} \Rightarrow A = \frac{n|\beta|^3}{\pi^{3/2}} \quad (*)$$

Ex: $\underline{\alpha} = \underline{u}$ using $\underline{u} = \frac{1}{n}\int_{\mathbb{R}^3} \underline{c} f(\underline{c})\,d\underline{c}$

Also, $$\frac{3}{2}k_B T = \frac{m}{2} A \int_{\mathbb{R}^3} \xi^2 e^{-\beta^2\xi^2}\,d\underline{\xi}$$

$$3k_B T = mA \int_0^{4\pi}\int_0^{\pi}\int_0^{\infty} \xi^4 e^{-\beta^2\xi^2} \sin\psi\, d\psi\, d\phi\, d\xi$$

$$= mA \cdot 2\pi \cdot \int_0^{\pi} \sin\psi\, d\psi \int_0^{\infty} \xi^4 e^{-\beta^2\xi^2} d\xi$$

$$= 2 \qquad = I_4 = \frac{3}{8}\frac{\sqrt{\pi}}{|\beta|^5}$$

using $(*)$

$$\beta^2 = \frac{m}{2k_B T}$$

$$A = \frac{n}{(2\pi RT)^{3/2}} \qquad k_R = \frac{RM}{N_A} = Rm$$

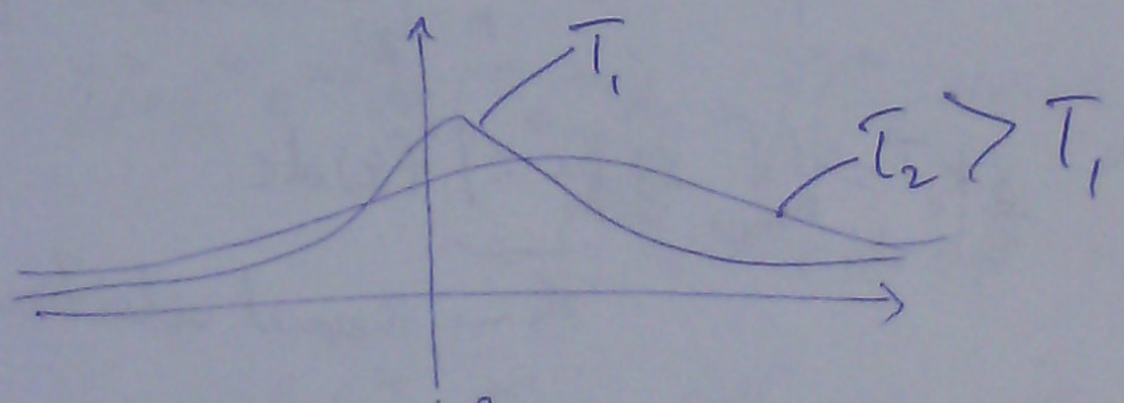
Maxwell - Boltzmann distribution

$$f(\underline{c}) = \frac{n}{(2\pi RT)^{3/2}} e^{-\frac{|\underline{c}-\underline{u}|^2}{2RT}} \qquad \hat{f} = \frac{1}{n} f$$

compare to standard Gaussian

$$N^3(\mu,\sigma) = \frac{1}{(2\pi)^{3/2}\sigma^3} f^{-\frac{|\underline{x}-\underline{\mu}|^2}{2\sigma^2}}$$

$$\sigma^2 = RT \qquad \mu_i = u_i \quad i = 1,2,3$$



4/11 (4.2) Equilibrium velocity distribution

(i) basic definitions

Postulate $\hat{f}(\underline{c})$ molecular velocities s.t.

$$\int_{\mathbb{R}^3} \hat{f}(\underline{c})\,dc_1 dc_2 dc_3 = 1$$

$d\underline{c}$

Hence $\hat{f}(\underline{c})d\underline{c}$ is probability that molecule has velocity components between $c_i < C_i + dc_i$ $i = 1,2,3$

Winter Semester 2016/17

Lattice-Boltzmann Methods

Prof. Georg May

Tutorial 3

Problem 1

Derive an expression for the thermodynamic pressure as the mean flux of the molecular "thermal" momentum $m\boldsymbol{\xi}$. (Here $\boldsymbol{\xi} = \mathbf{c} - \mathbf{u}$ is the thermal vecocity, given by the difference between the molecular velocity $\mathbf{c}$ and the bulk fluid velocity $\mathbf{u}$.)

Problem 2

Compute the mean velocity *magnitude* for a gas in thermodynamic equilibrium from the Maxwell-Boltzmann distribution.

Problem 3

Compute the mean free path of a molecule of a gas in thermodynamic equilibrium, using the Maxwell-Boltzmann distribution.

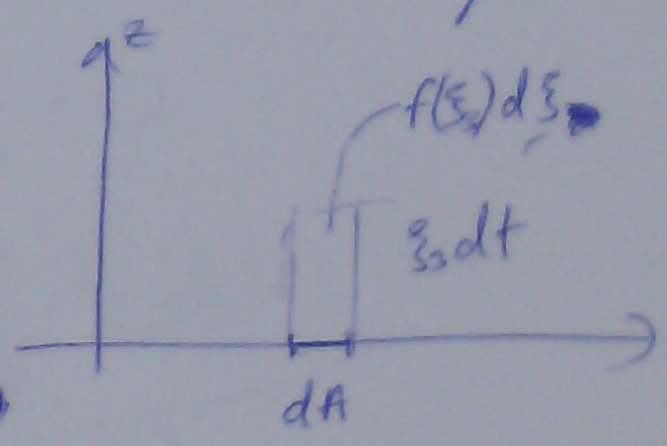
1) Pressure $[p] = \frac{[F]}{[A]} = \frac{[mv]}{[t]} \cdot \frac{1}{[A]}$ ← Momentum

thermal velocity $\underline{\xi} = \underline{c} - \underline{u}$

we define pressure as mean momentum flux of thermal momentum

$$m\underline{\xi} = m(\xi_1, \xi_2, \xi_3)^T$$

Assume equilibrium → f is Maxwellian



momentum $dM = m\,\xi_3^2\, f(\xi_3)\, dt\, dA\, d\xi_3$

$$p_3 = \iiint m\,\xi_3^2\, f(\xi_3)\, d\xi_3\, d\xi_2\, d\xi_1$$

$$p = \frac{1}{3}(p_1 + p_2 + p_3) = \frac{1}{3}\cdot 2 \int \frac{m}{2} |\xi|^2 f(\xi_3)\, d\underline{\xi} = \frac{2}{3}\frac{5}{2} n k_B T$$

$$\underline{p = n k_B T}$$

2) $\hat{f} = \frac{1}{n} f \qquad \hat{f}(c) = \frac{1}{(2\pi RT)^{3/2}} \int_{\mathbb{R}^3} e^{-\frac{|c|^2}{2RT}} dc \qquad (u=0)$

$$\bar{c} = \frac{1}{(2\pi RT)^{3/2}} \int_{R^3} |c| e^{-\frac{|c|^2}{2RT}} dc$$

spherical coordinates

$$= \frac{1}{(2\pi RT)^{3/2}} \int_0^{\infty}\int_0^{\pi}\int_0^{2\pi} c^3 e^{-\frac{c^2}{2RT}} \sin\psi \, d\psi \, d\phi \, dc$$

$$\frac{4\pi}{(2\pi RT)^{3/2}} I_3\left(\frac{1}{2RT}\right)$$

$$\frac{1}{2\left(\frac{1}{2RT}\right)^2} = 2(RT)^2$$

$$\bar{c} = \sqrt{\frac{8RT}{\pi}}$$

Speed of sound $c = \sqrt{\gamma RT}$ $\gamma = 5/3$ for monoatomic

3) $\frac{dV}{dt} = \frac{1}{n}\int_{\mathbb{R}^1} \left|\frac{\partial f(\underline{c}) d\underline{c}}{\partial t}\right|_{(1)}$ (frequency)

$$= \frac{1}{n} \int_{A_c}\int_{\mathbb{R}^3}\int_{\mathbb{R}^3} g(c,\xi) f(\underline{c}) f(\underline{\xi}) \, dA_c \, d\underline{\xi} \, d\underline{c}$$

$dA_c = d^2 \sin\psi \cos\psi \, d\varepsilon \, d\psi$

$$= \frac{1}{n} \frac{n^2 d^2}{(2\pi RT)^3} \int_{R^3}\int_{R^3}\int_0^{2\pi}\int_0^{\pi/2} g(c,\xi) e^{-\frac{|c|^2+|\xi|^2}{2RT}} \sin\psi\cos\psi \, d\psi \, d\varepsilon \, dc \, d\xi$$

$$\nu = \frac{nd^2}{(2\pi RT)^3} \pi \iint_{R^3 R^3} g(\underline{c},\underline{\xi}) e^{-\frac{|c|^2+|\xi|^2}{2RT}} dc \, d\xi$$

$$\underline{g} = \underline{\xi} - \underline{c} \quad , \quad \underline{w} = \frac{1}{2}(\underline{\xi}+\underline{c}) = \frac{1}{2}(\underline{g}+2\underline{c})$$

$$\underline{\xi} = \underline{g} + \underline{c} = \underline{w} + \frac{1}{2}\underline{g} \; ; \quad \underline{c} = \underline{w} - \frac{1}{2}\underline{g}$$

$$\nu = \frac{\pi n d^2}{(2\pi RT)^3} \iint_{R^3 R^3} g \, e^{-\frac{|w|^2+\frac{1}{4}|g|^2}{2RT}} dw \, dg$$

$$\int_{R^3} g \, e^{-\frac{g^2}{4RT}} dg \qquad \int_{R^3} e^{-\frac{w^2}{2RT}} dw$$

$$(4\pi)\int_0^{\infty} g^3 e^{-\frac{g^2}{4RT}} dg \qquad \int_0^{\infty} w^2 e^{-\frac{w^2}{2RT}} dw$$

$$8RT \qquad \frac{(\pi RT)^{3/2}}{4\pi}$$

$$\nu = 4n d^2 \sqrt{\pi RT}$$

time bet. collisions $= \tau = 1/\nu$

$$\lambda = \bar{c}\,\tau = \frac{1}{\sqrt{2}\pi n d^2}$$

Take moments of Boltzmann eqn's

$$\int_{\mathbb{R}^3} \phi(c) \left\{ \frac{\partial f}{\partial t} + c_\alpha \frac{\partial f}{\partial x_\alpha} - J(f,f) \right\} dc = 0$$

(i) $\phi(c) = m$

$$\int_{\mathbb{R}^3} m \left\{ \frac{\partial f}{\partial t} + c_\alpha \frac{\partial f}{\partial x_\alpha} \right\} dc = 0$$

$$\frac{\partial}{\partial t}\underbrace{\left(m \int_{\mathbb{R}^3} f(c)\, dc\right)}_{n} + \frac{\partial}{\partial x_\alpha} \underbrace{m \int_{\mathbb{R}^3} c_\alpha f(c)\, dc}_{n u_\alpha} = 0$$

$$\frac{\partial}{\partial t}(\rho) + \frac{\partial (\rho u_\alpha)}{\partial x_\alpha} = 0$$

(ii) $\phi(c) = m c_\alpha$

$$= \int_{\mathbb{R}^3} m c_\alpha \left(\frac{\partial f}{\partial t} + c_\beta \frac{\partial f}{\partial x_\beta} \right) dc = 0$$

$$\frac{\partial}{\partial t} \underbrace{m \int_{\mathbb{R}^3} c_\alpha f\, dc}_{n u_\alpha} + \frac{\partial}{\partial x_\beta} m \int_{\mathbb{R}^3} c_\alpha c_\beta f(c)\, dc = 0$$

$c = u + \xi$

$$\frac{\partial}{\partial t}(\rho u_\alpha) + \frac{\partial}{\partial x_\beta} m \int_{\mathbb{R}^3} (u_\alpha + \xi_\alpha)(u_\beta + \xi_\beta) f(\xi)\, d\xi$$

$$\frac{\partial}{\partial t}(\rho u_\alpha) + \frac{\partial}{\partial x_\beta} m \left\{ \underbrace{\int_{\mathbb{R}^3} u_\alpha u_\beta f(c)\, dc}_{n u_\alpha u_\beta} + \int_{\mathbb{R}^3} \xi_\alpha u_\beta \tilde{f}(\xi)\, d\xi + \int_{\mathbb{R}^3} u_\alpha \xi_\beta \tilde{f}(\xi)\, d\xi + \underbrace{\int_{\mathbb{R}^3} \xi_\alpha \xi_\beta \tilde{f}(\xi)\, d\xi}_{\frac{P_{\alpha\beta}}{m}} \right\} = 0$$

(iii) $\phi(c) = \frac{1}{2} m c^2 \qquad c = |c|$

$$\int_{\mathbb{R}^3} \frac{1}{2} m c^2 \left\{ \frac{\partial f}{\partial t} + c_\alpha \frac{\partial f}{\partial x_\alpha} \right\} dc = 0$$

$$\underbrace{\frac{\partial}{\partial t} \frac{1}{2} m \int_{\mathbb{R}^3} c^2 f(c)\, dc}_{(a)} + \underbrace{\frac{\partial}{\partial x_\alpha} \frac{1}{2} m \int_{\mathbb{R}^3} c^2 c_\alpha f(c)\, dc}_{(b)} = 0$$

(1)

Note $c^2 = (u + \xi, u + \xi) = u^2 + 2(\xi, u) + \xi^2$

$$(a) = \frac{\partial}{\partial t} \frac{m}{2} \int_{\mathbb{R}^3} (u^2 + \xi^2) f(\xi)\, d\xi = \frac{d}{dt}\left(\frac{1}{2} \rho u^2 + \underbrace{\int_{\mathbb{R}^3} \frac{m}{2} \xi^2 f(\xi)\, d\xi}_{= \frac{3}{2} n k_B T} \right)$$

$$= \frac{d}{dt} E \qquad E$$

(b) $\frac{\partial}{\partial x_\beta}\left\{\frac{m}{2}\int_{\mathbb{R}^3}(\xi_\beta+u_\beta)(u^2+2(\xi_\alpha u_\alpha+\xi^2)f(\xi)d\xi\right.$

$\frac{\partial}{\partial x_\beta}\left\{\underbrace{\frac{m}{2}\int_{\mathbb{R}^3} 2\xi_\alpha\xi_\beta u_\alpha f(\xi)d\xi}_{P_{\alpha\beta}u_\alpha} + \underbrace{\frac{m}{2}\int_{\mathbb{R}^3}\xi_\beta\xi^2 f(\xi)d\xi}_{q_\beta} + \underbrace{\frac{m}{2}u^2u_\beta\int_{\mathbb{R}^3}f(\xi)d\xi + \frac{m}{2}u_\beta\int_{\mathbb{R}^3}\xi^2 f(\xi)d\xi}_{Eu_\beta}=0\right.$

(a)+(b) $\Rightarrow \frac{\partial E}{\partial t}+\frac{\partial}{\partial x_\beta}(Eu_\beta)+\frac{\partial}{\partial x_\beta}(P_{\alpha\beta}x_\alpha)+\frac{\partial q_\beta}{\partial x_\beta}=0$

Assume local thermodynamic equilibrium

$$f(\xi,x,t)=\frac{n(x,t)}{(2\pi RT(x,t))^{3/2}}e^{-\frac{|c-u(x,t)|^2}{2RT(x,t)}}$$

Consider $P_{\alpha\beta}=\int_{\mathbb{R}^3}m\xi_\alpha\xi_\beta f(\xi)d\xi=\underbrace{\frac{\rho}{nM(2\pi RT)^{3/2}}}_{A}\int_{\mathbb{R}^3}\xi_\alpha\xi_\beta e^{-\frac{\xi_1^2+\xi_2^2+\xi_3^2}{2RT}}d\xi$

(i) $\underline{\alpha\neq\beta}$ $P_{\alpha\beta}=A\int_{\mathbb{R}^3}\xi_\alpha e^{-\frac{\xi_\alpha^2}{2RT}}d\xi\int_{\mathbb{R}^3}d\xi_\beta\,\xi_\beta e^{-\frac{\xi_\beta^2}{2RT}}\int_{\mathbb{R}^3}e^{-\frac{\xi_\gamma^2}{2RT}}d\xi$ ($\to 0$)

$\alpha,\beta,\gamma=\sigma(1,2,3)$

$P_{\alpha\beta}=0 \quad \alpha\neq\beta$

(ii) $\alpha=\beta$ $P_{\alpha\alpha}=\frac{A}{\quad}\int_{\mathbb{R}^3}m\xi_\alpha^2 e^{-\frac{\xi_1^2+\xi_2^2+\xi_3^2}{2RT}}d\xi \qquad \alpha=1,2,3$

$=\underbrace{\frac{A}{3}\int_{\mathbb{R}^3}m(\xi_1^2+\xi_2^2+\xi_3^2)e^{-\frac{\xi^2}{2RT}}d\xi}_{P}$

$P_{\alpha\beta}=P\delta_{\alpha\beta}$

$q_\beta=\int\frac{m}{2}\xi^2\xi_\beta f(\xi)d\xi=\frac{\rho}{(2\pi RT)^{3/2}}\int_{\mathbb{R}^3}\xi^2\xi_\beta e^{-\frac{\xi^2}{2RT}}d\xi$

Spherical coordinates

$q_\beta=A\int_0^{2\pi}\int_0^{\pi}\int_0^{\infty}\xi^2\xi_\beta\cdot h(\psi,\phi)e^{-\frac{\xi^2}{2RT}}\xi^2\sin\psi\,d\psi\,d\phi\,d\xi$

$h(\psi,\phi)=\begin{pmatrix}\sin\psi\cos\phi\\ \sin\psi\sin\phi\\ \cos\psi\end{pmatrix}$

$q_\beta=A\int_0^\infty\xi^5 e^{-\frac{\xi^2}{2RT}}d\xi\int_0^{\pi}\int_0^{2\pi}h(\psi,\phi)\sin\psi\,d\psi\,d\phi$

$\beta=1$ $\int_0^{2\pi}\cos\phi\,d\phi=0$

$\beta=2$ $\int_0^{2\pi}\sin\phi\,d\phi=0$

$\beta=3$ $\int_0^{\pi}\sin\psi\cos\psi=\frac{1}{2}\sin^2\psi\Big|_0^{\pi}=0$

$\Big\}\to q_\beta=0$

$$\Rightarrow \frac{\partial \rho}{\partial t} + \frac{\partial(\rho u_\alpha)}{\partial x_\alpha} = 0$$

$$\frac{\partial \rho u_\alpha}{\partial t} + \frac{\partial(\rho u_\alpha u_\beta)}{\partial x_\beta} + \frac{\partial P}{\partial x_\alpha} = 0$$

$$\frac{\partial E}{\partial t} + \frac{\partial E u_\beta}{\partial x_\beta} + \frac{\partial P u_\beta}{\partial x_\beta} = 0$$

f is locally maxwellian

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Collisional Invariants

collision integral

$$J(f,f) = \int_{\mathbb{R}^3}\int_{A_c} g(\underline{c},\underline{z})\left(f(\underline{c}')f(\underline{z}') - f(\underline{c})f(\underline{z})\right) d\underline{z}\, dA_c$$

$$\begin{pmatrix} c' \\ z' \end{pmatrix} : F = \begin{pmatrix} F_1(\underline{c},\underline{z},\psi,\varepsilon) \\ F_2(\underline{c},\underline{z},\psi,\varepsilon) \end{pmatrix} \qquad \begin{aligned} F_1 &= \underline{c} + 2\mu_B(g, k(\psi,\varepsilon))\, k(\psi,\varepsilon) \\ F_2 &= \underline{z} - 2\mu_A(g, k(\psi,\varepsilon))\, k(\psi,\varepsilon) \end{aligned}$$

$$\mu_A = \mu_B = 1/2$$

consider Moments

$$\underline{I}_\phi = \int_{\mathbb{R}^3} J(f,f)\,\phi(\underline{c})\, d\underline{c}$$

(1) $$\underline{I}_\phi = \int_{\mathbb{R}^3}\int_{\mathbb{R}^3}\int_{A_c} g(c,z)\left(f(\underline{c}')f(\underline{z}') - f(\underline{c})f(\underline{z})\right)\phi(c)\, d\underline{c}\, d\underline{z}\, dA.$$

$\underline{c} \leftrightarrow \underline{z}$

$$\underline{I}_\phi = \int_{\mathbb{R}^3}\int_{\mathbb{R}^3}\int_{A_c} g(\underline{z},\underline{c})\left(f(\underline{c}'')^{(2,c')} f(\underline{z}'')^{(1,c)} - f(\underline{c})f(\underline{z})\right)\phi(\underline{z})\, d\underline{z}\, d\underline{c}\, dA_c$$

Now consider physical symmetries

$$g(\underline{c},\underline{z}) = -g(\underline{z},\underline{c})$$

$$g(c,z) = g(z,c)$$

$$\underline{c}'(\underline{c},\underline{z}) = \underline{z}'(\underline{z},\underline{c}) \qquad \underline{z}'(\underline{c},\underline{z}) = \underline{c}'(\underline{z},\underline{c})$$

(1)

(2) $$\underline{I}_\phi = \int_{\mathbb{R}^3}\int_{\mathbb{R}^3}\int_{A_c} g(c,z)\left(f(\underline{c}')f(\underline{z}') - f(\underline{c})f(\underline{z})\right)\phi(z)\, d\underline{c}\, d\underline{z}\, dA_c$$

(c,z)

$$\underline{I}_\phi = \frac{1}{2}\left(\underline{I}_{\phi(1)} + \underline{I}_{\phi(2)}\right)$$

Similarly we can write

$$\underline{I}_\phi = \frac{1}{4}\int_{\mathbb{R}^3}\int_{\mathbb{R}^3}\int_{A_c} g(\underline{c},\underline{z})\left(f(\underline{c}')f(\underline{z}') - f(\underline{c})f(\underline{z})\right)\left(\phi(\underline{c}) + \phi(\underline{z}) - \phi(\underline{c}') - \phi(\underline{z}')\right) d\underline{c}\, d\underline{z}\, dA_c$$

(8.3) Analysis of LGA

(8.3.1) The collision operator

$$n_i'(r,t) = n_i(r,t) + \Delta_i(r,t)$$

$$\Delta_i \in \{-1, 0, 1\}$$

Remark: In the following

$$i+k = \begin{cases} i+k & \text{if } i+k < 6 \\ i+k-6 & \text{if } i+k \geq 6 \end{cases} \quad \text{mod}$$

Derive an algebraic expression for Δ_i

Then $\Delta = (\Delta_i)_{i=0,\dots,5}$

Consider binary collision (Type A)

	n_i	n_{i+1}	n_{i+2}	n_{i+3}	n_{i+4}	n_{i+5}
Case 1	1	0	0	1	0	0
Case 2	0	1	0	0	1	0
Case 3	0	0	1	0	0	1

$$\delta_i^{(A,1)} = n_i\, n_{i+3} (1-n_{i+1})(1-n_{i+2})(1-n_{i+4})(1-n_{i+5})$$

$$\delta_i^{(A,2)} = n_{i+1}\, n_{i+4} (1-n_i)(1-n_{i+2})(1-n_{i+3})(1-n_{i+5})$$

$$\delta_i^{(A,3)} = \text{---}$$

Collisim operator is constructed

$$\Delta_i^{(A)} = a_1 \delta_i^{(A,1)} + a_2 \delta_i^{(A,2)} + a_3 \delta_i^{(A,3)}$$

$$a_1 = -1 \qquad a_2 = \xi \qquad \xi = \{0, 1\} \text{ random bit}$$

$$a_3 = 1 - \xi$$

$$\Rightarrow \Delta_i^{(A)} = -\delta_i^{(A,1)} + \xi\, \delta_i^{(A,2)} + (1-\xi)\, \delta_i^{(A,3)}$$

Consider 3-way collision (B)

$$\delta_i^{(B,1)} = n_i\, n_{i+2}\, n_{i+4} (1-n_{i+1})(1-n_{i+3})(1-n_{i+5})$$

$$\delta_i^{(B,2)} = n_{i+1}\, n_{i+3}\, n_{i+5} (1-n_i)(1-n_{i+2})(1-n_{i+4})$$

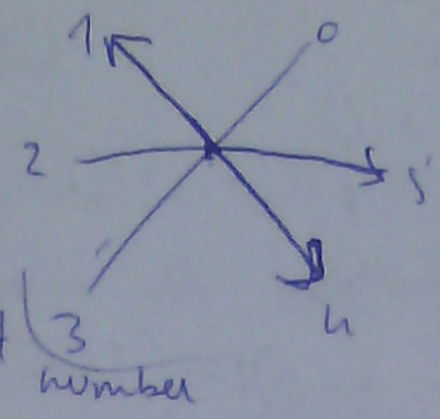
$$\Delta_i^{(B)} = -\delta_i^{(B,1)} + \delta_i^{(B,2)}$$

$$\Delta_i = \Delta_i^{(A)} + \Delta_i^{(B)} \left(+ \Delta_i^{(C)} + \Delta_i^{(D)}\right)$$

11/12 Implementation of LGA

(1) Preliminaries

$n = (110010)$



- In practical: Use 8 b.f (3 number)
- possible datatypes

C: ~~oooo~~ unsigned char (int8_t (c99))

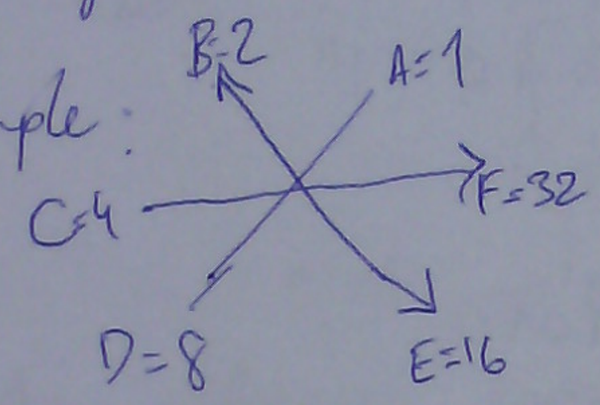
Matlab: uint8

Fortran (90+): INTEGER(1)

Algebraic vs logical method

i.e integer arithmetic or boolean operators

Example:



$n = (110010)$

$= 2^5 + 2^4 + 2$

$= (50)_{10}$

set state as $n = B + E + F$ 'Algebraic'

or $n = \underbrace{(1<<1)}_{B} | \underbrace{(1<<4)}_{E} | \underbrace{(1<<5)}_{F}$ bit shift

$= (000010) | (010000) | (100000)$ OR

$= (110010)_2$

Initialization

Start with $\sum_{i=0}^{5} N_i = : S \qquad S \in [0,1]$

average $\langle n_i \rangle$

(i) Algebraic method

Set $S = S_0 \in [0,1]$

for $s = 1, \ldots N_s$ — No of nodes

$n = (r_{s,t=0}) = 0$

for $k = 0, \ldots, 5$

if $\lfloor rand + S_0 \rfloor$ — floor / integer part

$n_k (r_s, t=0) += c_k$

end end if

end end

rand → random no $\in (0,1)$

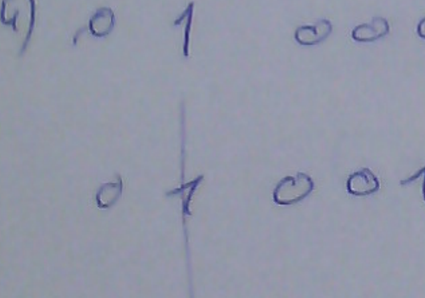
(ii) boolean operations

```
for s = 1, ... N_s
    n(r_s, t=0) = 0
    for k = 0, 1 --- 5
        if [rand + S_0]
            n_k(r_s, t=0) |= (1<<k)
        end if
    end
end
```

Collision implemented using look-up table

Index			value
B	E	State (6-bits)	
0	0	000000	000000
0	0	000001	000001
0	0	000010	000010
		⋮	⋮
$(9)_{10}$ 0	0	001001	010010
		⋮	⋮
(21) 0	0	010101	101010
		⋮	
(63) 0	0	111111	111111
(64) 0	1	000000	000000
		⋮	⋮
0	1	001001	100100
		⋮	⋮
(127) 0	1	111111	111111
128 1	0	000000	

Boundary conditions



Define: Let pA be neighbour in direction A

$n(pA) \mid = \underbrace{n'(z)}_{\text{State after collision}} \& A$

$n(pB) \mid = n'(z) \& B$

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LGA Analysis

The collision operator

$$\Delta_i(n) = n_i'(n) - n_i$$

$$n = (n_5 n_4 n_3 n_2 n_1 n_0)$$

$$n_0 n_3 (1-n_1)(1-n_2)(1-n_4)(1-n_5) = \begin{cases} 1 & \text{if } (n = 001001) \\ 0 & \end{cases}$$

Generalized expression for identifying a^{th} state

set

$$S = \{0,1\}^5 = \{0,1\} \times \{0,1\} \times \cdots \times \{0,1\}$$

$$= \{(s_5 s_4 \cdots s_0) : s_i \in \{0,1\} \quad i = 0,1,\ldots 5\}$$

$$\# S = 64$$

Note. For $n_j, s_j \in \{0,1\}$

$$n_j^{s_j}(1-n_j)^{1-s_j} = \begin{cases} 1 & \text{if } n_j = s_j \\ 0 & n_j \neq s_j \end{cases}$$

check

$$n_j = 0 \cdot \begin{cases} s_j = 0 : 0^0 1^1 = 1 \\ s_j = 1 : 0^1 1^0 = 0 \end{cases}$$

$n_j = 1 \rightarrow$ similar

Define 'algebraic' Kronecker delta

$$\delta_{n,s} = \prod_{j=0}^{5} n_j^{s_j}(1-n_j)^{1-s_j} = \begin{cases} 1 & n = s \\ 0 & n \neq s \end{cases}$$

Transition b/t

For each $s, s' \in S$ 'transition b/t'

$$\xi_{s,s'} = \begin{cases} 1 & s' \leftarrow\!\!\!\!\!\!\rightarrow s \\ 0 & \text{otherwise} \end{cases}$$ connected by admissible collision @ (δ, t)

Note: This will be set such that $\langle \xi_{s,s'} \rangle$ is the correct probability (probabilities) for transition between $s \& s'$

$$\sum_{s' \in S} \langle \xi_{s,s'} \rangle = 1$$

$$\sum_{s' \in S} \xi_{s,s'} = 1$$

Given input state n, output state is

$$n_i'(n) = \sum_{s \in S^\bullet} \sum_{s' \in S^e} s_i' \, \xi_{s,s'} \underbrace{\prod_{j=0}^{5} n_j^{s_j}(1-n_j)^{1-s_j}}_{\delta_{n,s}}$$

$$n_i = \sum_{s \in S} s_i \delta_{n,s} = \sum_{s'} \sum_{s} s_i \delta_{n,s} \xi_{s,s'}$$

$\delta_{n,s}$

$$\Delta_i(n) = \sum_{s,s'} (s_i' - s_i)\, \xi_{ss'} \prod_{j=0}^{5} n_j^{s_j} (1-n_j)^{1-s_j}$$

	Kinetic Theory	Lattice Methods
micro-dynamics	Eqn of motion for each particle	LGA
stochastic description	Distribution function $f(c,x,t)$ Equilibrium (MB)	MB for discrete LGA (Today)
	Non-equilibrium: Boltzmann eq.	'averaged' LGA → Lattice Boltzmann Method
Macroscopic (Conservation laws)	Moment> + Chapman-Enskog	(Discrete) moments + multiscale expansion

Equilibrium Solution of LGA

Postulate N_i: Probability of link i being occupied $= P(n_i = 1)$

Define $\rho = \sum_{i=0}^{5} N_i \qquad \underline{u} = \frac{1}{\rho} \sum_{i=0}^{5} \underline{c}_i N_i$

Statistically independent

$N_i N_j$: probability $P(n_i = 1 \;\&\; n_j = 1)$

Consider:

$$P(n=(1,1,1,1,1,1)) = \prod_{j=0}^{5} N_j$$

$$P(n=(0,0,0,0,0,0)) = \prod_{j=0}^{5} (1-N_j)$$

$$P(n=(1,1,1,0,0,0)) = \prod_{j=0}^{2} (1-N_j) \prod_{j=3}^{5} N_j$$

$$P(s) = \prod_{j=0}^{5} N_j^{s_j} (1-N_j)^{1-s_j}$$

$$P(s') = \prod_{j=0}^{5} N_j^{s_j'} (1-N_j)^{1-s_j'} = \sum_{s \in S} \langle \xi_{ss'} \rangle P(s)$$

$$\sum_{s' \in S} s_i' \left(P(s') = \prod_{j=0}^{5} N_j^{s_j'} (1-N_j)^{1-s_j'} = \sum_{s \in S} \langle \xi_{ss'} \rangle P(s) \right)$$

$$= \sum_{s,s' \in S} s_i' \prod_{j=0}^{5} N_j^{s_j'} (1-N_j)^{1-s_j'} = \sum_{s,s' \in S} s_i' \langle \xi_{ss'} \rangle \prod_{j=0}^{5} N_j^{s_j} (1-N_j)^{1-s_j}$$

No need of primes because they are summation index ⊗

Note $\sum_{s' \in S} \langle \xi_{ss'} \rangle = 1$

$$\sum_{s,s' \in S} (s_i' - s_i) \langle \xi_{ss'} \rangle \prod_{j=0}^{5} N_j^{s_j} (1-N_j)^{(1-s_j)} = 0 \Rightarrow \text{on average collision operator vanishes}$$

$i = 0, 1, 2 \ldots 5$

$$\Rightarrow \underbrace{\prod_{j=0}^{5}(1-N_j)}_{\neq 0}\Big(\sum_{s,s'\in S}(s_i'-s_i)\langle\xi_{ss'}\rangle \prod_{j=0}^{5}\underbrace{\left(\frac{N_j}{1-N_j}\right)^{s_j}}_{\eta_j}\Big)=0$$

$$= 0 \times \sum_{j=0}^{5}\log n_j$$

$$\sum_{i=0}^{5}\log n_i \sum_{s,s'\in S}(s_i'-s_i)\langle\xi_{ss'}\rangle \prod_{j=0}^{5}\left(\frac{}{1-\epsilon N_j}\right) n_j^{s_j} = 0$$

$$\sum_{s'\in S}\langle\xi_{ss'}\rangle\left(\sum_{i=0}^{5}(s_i'-s_i)\log\eta_i\right)\prod_{j=0}^{5}\eta_j^{s_j} = 0$$

$$\sum_{s,s'\in S}\langle\xi_{ss'}\rangle \log\left(\frac{\prod n_i^{s_i'}}{\prod n_j^{s_i}}\right)\prod_{j=0}^{5}\eta_j^{s_j} = 0$$

$$\prod_{j=0}^{5}\eta_j^{s_j} \to X_s$$

$$\sum_{s,s'\in S}\langle\xi_{ss'}\rangle \log\left(\frac{X_{s'}}{X_s}\right)X_s = 0 \quad \text{— (1)}$$

Note:

$$\sum_{s,s'\in S} X_s\langle\xi_{ss'}\rangle = \sum_{s} X_s \underbrace{\sum_{s'}\langle\xi_{ss'}\rangle}_{1} = \sum_{s'} X_{s'} \underbrace{\sum_{s}\langle\xi_{ss'}\rangle}_{=1?}$$

if no bias between states

$$= \sum_{ss'} X_{s'}\langle\xi_{ss'}\rangle$$

i.e.

$$\Rightarrow \sum_{s,s'}(X_s - X_{s'})\langle\xi_{ss'}\rangle = 0 \quad \text{— (2)}$$

$$-((1)+(2)) = 0$$

$$\sum_{ss'}\Big(-X_s\log\left(\frac{X_{s'}}{X_s}\right) + X_{s'} - X_s\Big)\underbrace{\langle\xi_{ss'}\rangle}_{\geq 0} = 0$$

$$\geq 0$$

$$\int_{X_{s'}}^{X_s}\log\left(\frac{t}{X_{s'}}\right)dt \geq 0$$

Case 1 $\langle\xi_{ss'}\rangle = 0$

Case 2 $\langle\xi_{ss'}\rangle \neq 0 \to s = s'$ ✓

$\hookrightarrow X_s = X_{s'}$ $(s' \neq s)$ $\prod_{i=0}^{5} n_i^{s_i} = \prod_{i=0}^{5} n_i^{s_i'} \Rightarrow \sum_{i=0}^{5}(s_i'-s_i)\log n_i = 0$

satisfied if $\log n_i = -(a + \underline{b}\cdot c_i)$

$$n_i = e^{-(a+\underline{b}\cdot c_i)} = \frac{N_i}{1-N_i}$$

$$1 - N_i = N_i e^{a+\underline{b}\cdot c_i}$$

$$\boxed{N_i = \frac{1}{1+e^{a+\underline{b}\cdot c_i}}}$$

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Recall: Maxwell Boltzmann

$$f(c) = A e^{-\beta^2 |c-\alpha|^2}$$

$$\left(\frac{\partial f}{\partial t}\right)_{coll} = 0$$

$$P(c) = \frac{1}{n}\int_{V_c} f(c)\,dc$$

use moments

$$n = \int_{\mathbb{R}^3} f(c)\,dc$$

$$n\underline{v} = \int_{\mathbb{R}^3} c f(c)\,dc$$

$$\frac{3}{2} n k_B T = \frac{m}{2}\int_{\mathbb{R}^3} (c-u)^2 f(c)\,dc$$

$\Rightarrow$ can express $A, \beta, \underline{\alpha}$ as func of $n, T, \underline{u}$

LGA

$$n_i(\underline{r}+\underline{c}_i, t+1) = n_i(\underline{r}, t) + \Delta_i(\underline{r}, t)$$

admits an equilibrium s.th $\langle \Delta_i \rangle = 0$

(1) $$\langle n_i \rangle = N_i^{eq} = \frac{1}{1+a e^{a+\underline{b}\cdot c_i}} \qquad i = 0, \dots, 5$$

(2) $$\rho = \sum_0^5 N_i^{eq}$$

(3) $$\rho \underline{u} = \sum_0^5 \underline{c}_i N_i^{eq}$$

cannot express $a, \underline{b}$ as func. of $\rho, \rho\underline{u}$

(1) Preliminary steps

Let $\underline{u} = (u_\alpha)_{\alpha=1,2}$

Set $a = a(\rho, u)$, $\underline{b} = \underline{b}(\rho, u)$

small velocity approximation

$$a(\rho, u) = \underbrace{a_0(\rho, 0)}_{a_0(\rho)} + \underbrace{\frac{\partial a}{\partial u_\alpha}\Big|_{(\rho,0)}}_{a_{1,\alpha}(\rho)} u_\alpha + \frac{1}{2}\underbrace{\frac{\partial^2 a}{\partial u_\alpha \partial u_\beta}\Big|_{(\rho,0)}}_{a_{2,\alpha\beta}(\rho)} u_\alpha u_\beta$$

$$a = a_0(s) + a_{1,\alpha} u_\alpha + a_{2,\alpha\beta} u_\alpha u_\beta + \dots$$

$$b_\alpha = b_{0,\alpha}(s) + b_{1\alpha\beta} u_\beta + b_{3\alpha\beta\gamma} u_\beta u_\gamma + \dots$$

Constraints

- At $u=0 \Rightarrow N_i = \text{const}\ \forall i$

  $\Rightarrow b_{0,\alpha} = 0 \quad \alpha = 1,2$

- Symmetry : N_i should be invariant under

  (i) coordinate reflection

  Let $x \to -x \quad (u \to -u \ , c_i \to -c_i)$

  $\Rightarrow a$: symmetric in $\underline{u}$

  b antisymmetric in $\underline{u}$

  $\Rightarrow a_{1,\alpha} = 0 \qquad b_{2,\alpha\beta\gamma} = 0$ ~~$\alpha=\beta$~~

  $\alpha, \beta, \gamma = 1, 2$

(ii) Isotropy

$$b_{1,\alpha\beta} = b_1 \delta_{\alpha\beta}$$

$$a_{2,\alpha\beta} = a_2 \delta_{\alpha\beta}$$

$$a = a_0(s) + a_2(s) u^2$$

$$b_\alpha = b_1 u_\alpha$$

Substitute (9) (N_i^{eq})

$$N_i^{eq} = \frac{1}{1 + e^{g_i(s,u)}} \qquad g_i = a_0(s) + a_2(s) u^2 + b_1 \underbrace{u_\alpha c_{i,\alpha}}_{\underline{u}\cdot\underline{c}_i}$$

(2) Expand N_i^{eq} in u

$$N_i^{eq} = \underbrace{N_i^{eq}(s,0)}_{(a)} + \underbrace{\left.\frac{\partial N_i^{eq}}{\partial u_\alpha}\right|_{s,0} u_\alpha}_{(c)} + \frac{1}{2}\left.\frac{\partial^2 N_i^{eq}}{\partial u_\alpha \partial u_\beta}\right|_{u=0} u_\alpha u_\beta + O(u^3)$$

(b)

(a) $N_i^{eq}(s,0) = \dfrac{1}{1+e^{a_0(s)}} = \dfrac{s}{6} = d$ (same for (2) all i)

(c) $\left(\frac{1}{1+e^x}\right)'_{x=a_0}$

$\left(e^{a_0} = \frac{1-d}{d}\right)$ eq (1)

(b) $(N_i^{eq})' \dfrac{\partial g_i}{\partial u_\alpha} =$ (i) (iii)

(c) $(N_i^{eq})'' \dfrac{\partial g_i}{\partial u_\alpha}\dfrac{\partial g_i}{\partial u_\beta} + (N_i^{eq})' \dfrac{\partial^2 g_i}{\partial u_\alpha \partial u_\beta} =$ (ii) (iv)

(i) $(N_i^{eq})'|_{u=0} = \frac{-e^{a_0}}{(1+e^{a_0})^2} = \cancel{(1-d)}\, d(d-1)$

(ii) $(N_i^{eq})''_{u=0} = \frac{e^{a_0}(e^{a_0}-1)}{(1+e^{a_0})^3} = d(d-1)(2d-1)$

(iii) $\left.\frac{dg_i}{du_\alpha}\right|_{u=0} = b_1 c_{i,\alpha}$

(iv) $\left.\frac{d^2 g_i}{\partial u_\alpha \partial u_\beta}\right|_{u=0} = 2a_2\delta_{\alpha\beta}$

$$N_i^{eq} = d + d(d-1)b_1 c_{i,\alpha}u_\alpha + \frac{1}{2}d(d-1)(2d-1)b_1^2 c_{i\alpha}c_{i\beta}u_\alpha u_\beta + \frac{1}{2}d(d-1)2a_2\delta_{\alpha\beta}u_\alpha u_\beta$$

$$\Rightarrow N_i^{eq} = d + d(d-1)b_1 c_{i,\alpha}u_\alpha + \frac{1}{2}d(d-1)\left\{(2d-1)b_1^2 c_{i,\alpha}c_{i,\beta} + 2a_2\delta_{\alpha\beta}\right\}u_\alpha u_\beta$$

$$S = \sum_{i=0}^{5} N_i^{(eq)} \qquad S\underline{u} = \sum_{i=0}^{5} c_i N_i^{eq}$$

Note: $\sum_{i=0}^{5} c_{i,\alpha} = 0 \qquad \sum_{i=0}^{5} c_{i\alpha}c_{i\beta} = 3\delta_{\alpha\beta}$

$$\Sigma c_{i\alpha}c_{i\beta}c_{i\delta} = 0$$

(2) $S = \Sigma N_i^{(eq)} = S + 0 + \frac{1}{2}d(d-1)\left\{12a_2\delta_{\alpha\beta} + 3(2d-1)b_1^2\delta_{\alpha\beta}\right\}u_\alpha u_\beta$

$$a_2 = \frac{(1-2d)b_1^2}{4}$$

(3) $S_{u_\beta} = \Sigma c_{i\beta}N_i^{eq} = d(d-1)b_1 \underbrace{\Sigma c_{i\alpha}c_{i\beta}}_{3\delta_{\alpha\beta}} u_\alpha \rightarrow 6d\,u_\beta$ ~~$6du$~~ u_β

$$b_1 = \frac{2}{d-1}$$

$$a_2 = \frac{(1-2d)}{(d-1)^2}$$

$$N_i^{(eq)} = d + 2d\,c_{i,\alpha}u_\alpha + \frac{d}{2(d-1)}\left(2(1-2d)\delta_{\alpha\beta} + (2d-1)4\,c_{i\alpha}c_{i\beta}\right)u_\alpha u_\beta$$

$$= d + 2d(\underbrace{\underline{c}_i \cdot \underline{u}_0}_{u_0(x)}) + \underbrace{\frac{2d(2d-1)}{d-1}}_{a_1,a'} \left(\underbrace{c_{i\alpha}c_{i\beta} - \tfrac{1}{2}\delta_{\alpha\beta}}_{a_2,\alpha\beta(x)}\right)u_\alpha u_\beta \rightarrow \frac{3}{3}\left(\frac{2\cdot 8 - 6}{5-6}\right)$$

$$G(s) = \frac{2s-6}{s-5}$$

$$N_i^{eq} = s\left(\frac{1}{6} + \frac{\underline{c}_i \cdot \underline{u}}{3} + \frac{1}{5} G(s) \delta_{\alpha\beta} u_\alpha u_\beta\right)$$

essarily (1)

9/12 LGA

$$n_i(\underline{r}+\underline{c}_i, t+1) = n_i'(\underline{r}, t)$$

Conservation $n_i'(r,t) = n_i(r,t) + \Delta_i(r,t)$

$$\sum_0^5 n_i' = \sum_0^5 n_i$$

$$\sum_0^5 \underline{c}_i n_i' = \sum_0^5 \underline{c}_i n_i$$

$N_i = \langle n_i \rangle$

$$\sum_{i=0}^5 N_i(\underline{r}, t) = \sum_0^5 \langle n_i \rangle = \sum_0^5 N_i(\underline{r}+\underline{c}_i, t+1) \quad \text{—(1)}$$

$$\sum \underline{c}_i N_i(\underline{r}, t) = \sum \underline{c}_i N_i(\underline{r}+\underline{c}_i, t+1) \quad \text{—(2)}$$

$$\rho = \sum_{i=0}^5 N_i \qquad \rho \underline{u} = \sum_0^5 \underline{c}_i N_i$$

Multiscale Expansion

Step 1 $N_i(\underline{r}, t) = N_i^{(0)} + \varepsilon N_i^{(1)} + \varepsilon^2 N_i^{(2)} + \cdots$

$\varepsilon = O(N^{-1})$

$$N_i^0 = N_i^{(eq)} = \frac{\rho}{6} + \frac{\rho}{3}(\underline{c}_i \cdot \underline{u}_i) + \frac{\rho}{3} G(\rho)\, Q_{i\alpha\beta} u_\alpha u_\beta$$

$\frac{2\rho - 6}{\rho - 6}$ $\quad Q_{i\alpha\beta} = c_{i\alpha} c_{i\beta} - \frac{1}{2}\delta_{\alpha\beta}$

$$\sum N_i^{eq} = \rho \quad \Rightarrow \sum_{i=0}^5 N_i^{(k)} = 0$$

$$\sum c_i N_i^{eq} = \rho \underline{u} \qquad \sum_{i=0}^5 \underline{c}_i N_i^{(k)} = 0 \quad k = 1, 2, 3 \ldots$$

Step 2

3 relevant time scales

$t = t^{(0)}$ "Noise"

$t^{(1)} = \varepsilon t$ "convection"

$t^{(2)} = \varepsilon^2 t$ "diffusion" $\varepsilon = O(N^{-1})$

multiscale modelling

$t^{(0)}$: averaged out

Assume $g(t^1(t), t^2(t))$

essarily (1)

$$\frac{\partial}{\partial t} = \partial_t = \frac{\partial}{\partial t^{(1)}} \frac{\partial t^{(1)}}{\partial t} + \frac{\partial}{\partial t^{(2)}} \frac{\partial t^{(2)}}{\partial t}$$

$$\frac{\partial}{\partial r_\alpha} = \partial_{r_\alpha} = \varepsilon \partial_{r_\alpha^{(1)}}$$

Step(3) Taylor Expansion

$$N_i(\underline{r}+\underline{c}_i, t+1) = N_i(r,t) + \varepsilon \partial_{r_\alpha^{(1)}} N_i c_{i,\alpha} + \varepsilon \partial_{t^1} N_i + \varepsilon^2 \partial_{t^{(2)}} N_i + O \cdots$$

higher order terms

$$N_i = N_i^{(0)} + \varepsilon N_i^1 + \varepsilon^2 N_i^{(2)}$$

Take Moments in (1) & collect terms

ε^1: $\partial_{t^{(1)}} \underbrace{\sum_{i=0}^{5} N_i}_{8} + \partial_{r_\alpha^{(1)}} \underbrace{\sum_{i=0}^{5} c_{i\alpha} N_i}_{8 q_\alpha u_\alpha} = 0$ Mass conservation

$\partial_{t^{(2)}} \sum_{i=0}^{5} N_i = 0$ ~~Stoc~~ vis

No viscous term in mass conservation

Problems with LGA.

- Noise problem
- Inconsistency in momentum ~~Poss~~ equations
- Viscosity
- complexity 2^b → no. of links

From LGA to LBM

LGA $n_i(r_i + c_i, t+1) = n_i(r,t) + \Delta_i(r,t)$

$$\Delta_i = \sum_{s,s' \in S} (s_i' - s_i) \underbrace{\xi_{s,s'}}_{\text{transition bit}} \underbrace{\prod_{j=0}^{5} n_j^{s_j} (1-n_j)^{1-s_j}}_{\partial_{n,s}} \quad (3')$$

$N_i = \langle n_i \rangle$

Step 1 Averaging the LGA

$\langle n_i(r+c_i, t+1) \rangle = \langle n_i(r,t) \rangle + \langle \Delta_i(r,t) \rangle$

$N_i(r+c_i, t+1) = N_i(r,t) + \langle \Delta_i(r,t) \rangle$

Split $n_i = \underbrace{\langle n_i \rangle}_{N_i} + \hat{n}_i$

$\langle \hat{n}_i \rangle = 0$

Substitute into (3)

$$\langle \Delta_i \rangle = \left\langle \sum_{s,s' \in S} (s_i' - s_i) \xi_{s,s'} \prod_{j=0}^{5} (N_j + \hat{n}_j)^{s_j} (1 - N_j - \hat{n}_j)^{1-s_j} \right\rangle$$

Note: we get terms like $\langle (N_i + \hat{n}_i)(N_j + \hat{n}_j) \rangle$

$= N_i N_j + \underbrace{\langle N_i \hat{n}_j \rangle + \langle N_j \hat{n}_i \rangle}_{0} + \langle \hat{n}_i \hat{n}_j \rangle$

Neglect $\langle n_i n_j \rangle$

$$N_i(r+c_i, t+1) = N_i(r,t) + \underbrace{\sum_{s,s' \in S} (s_i' - s_i) \xi_{s,s'} \prod_{j=0}^{5} N_j^{s_j} (1-N_j)^{1-s_j}}_{G(N_0, N_1, N_2, N_3, N_4, N_5)}$$

$G_i(N_0, N_1, N_2, N_3, N_4, N_5) = 0$

$a_{1,\alpha\beta}$ $a_{2,\alpha\beta\gamma}$

Summary
+ Noise removed
− now susceptible to round-off errors
− increased storage requirement
− everything else (complexity 2^b)

Step 2 Linearizing collision operator

Denote $N_i^{(eq,0)} = N_i^{(eq)}|_{n=0}$

Linearize around $N_i^{(eq,0)}$

(4) $C_i(N) = C_i(N^{(eq,0)}) + \frac{\partial C_i}{\partial N_j}\Big|_{u=0}(N_j - N_j^{(eq)}) + \frac{1}{2}\frac{\partial^2 C_i}{\partial N_j \partial N_k}(N_j - N_j^{(eq,0)})(N_k - N_k^{(eq,0)}) + \dots$

(5) $0 = C_i(N^{eq}) = C_i(N^{eq,0}) + \frac{\partial C_i}{\partial N_j}\Big|_{u=0}(N_j^{(eq)} - N_j^{(eq,0)}) + \frac{1}{2}\frac{\partial^2 C_i(N^{(1)})}{\partial N_j \partial N_k}() + \dots$

(4) − (5) → neglect

$$C_i \approx \frac{\partial C_i}{\partial N_j}(N_j - N_j^{(eq)}) + \dots$$

$$\frac{\partial C_i}{\partial N_j} \leq \begin{pmatrix} \frac{\partial C_0}{\partial N_0} & \cdots & \frac{\partial C_0}{\partial N_5} \\ \vdots & & \vdots \\ \frac{\partial C_5}{\partial N_0} & \cdots & \frac{\partial C_r}{\partial N_5} \end{pmatrix}$$

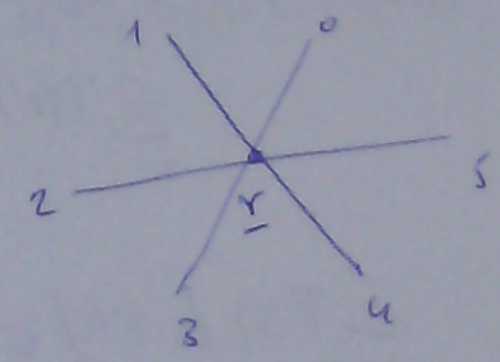
$$N_i(\underline{r} + \underline{c}_i, t+1) = N_i(\underline{r}, t) + \left(\frac{\partial C_i}{\partial N_j}\right)(N_j - N_j^{(eq)})$$

Note: Complexity now b^2 (before 2^b)

15/12

H-Theorem for LGA

$n = (n_i)_{i=0,\dots,5}$ where $n_i \in \{0,1\}$



$N_i = \langle n_i \rangle = P(n_i = 1)$

$1 - N_i = P(n_i = 0)$

Equilibrium:

$$P(s \in S') = \prod_{j=0}^{5} N_j^{s_j}(1-N_j)^{1-s_j} \quad (1) \quad s \in \{0,1\}^6$$

$P(s = 111000) = N_5 N_4 N_3 (1-N_2)(1-N_1)(1-N_0)$

Let $P(s)$ be general probability of state $s \in S'$ not necessarily (1)

$$\sum_{s \in S} P(s) = 1$$

$$N_i = \sum_{s \in S} s_i P(s)$$

$$1 - N_i = \sum_{s \in S} (1 - s_i) P(s)$$

consistency with N-S

Now probability of $s' \in S$ after collision (time t')

$$P'(s') = \sum_{s \in S'} \langle \xi_{ss'} \rangle P(s)$$

$P(s', t')$ $\qquad$ $P(s, t)$

$$\sum_{s' \in S} \langle \xi_{ss'} \rangle = 1 \qquad (2)$$

$$\sum_{s \in S} \langle \xi_{ss'} \rangle = 1 \qquad (3)$$

Proposition:

for any convex function f,

$$\sum_{s'} f(P'(s')) \leq \sum_{s} f(P(s))$$

Proof: Note f convex $\rightarrow f(\xi x_1 + (1-\xi) x_2) \leq \xi f(x_1) + (1-\xi) f(x_2)$

Also holds for convex combination of n variables $\quad \xi \in [0,1]$

$$f\left(\sum_{i=1}^{n} \xi_j x_j\right) \leq \sum_{i=1}^{n} \xi_j \cdot f(x_j) \qquad \sum_{j=1}^{n} \xi_j = 1$$

$$f\left(\sum_{s \in S} \langle \xi_{ss'} \rangle P(s)\right) \leq \sum_{s \in S} \langle \xi_{ss'} \rangle f(P(s))$$

Sum over all $s' \in S$

$$\sum_{s' \in S} f(P'(s')) \leq \sum_{s' \in S} \sum_{s \in S} \langle \xi_{ss'} \rangle f(P(s))$$

$$= \sum_{s \in S} f(P(s))$$

Let $f(x) = x \ln x$

$$\sum_{s'} P'(s') \ln(P'(s')) \leq \underbrace{\sum_{s} P(s) \ln P(s)}_{H(s,t)}$$

$$\sum_{s \in S} P(s) \ln P(s) \leq \sum_{i=0}^{r} N_i \ln N_i + (1-N_i) \ln(1-N_i) \qquad (4)$$

with equality iff $\qquad (*)$

$$P(s) = \prod_{i=0}^{r} N_i^{s_i} (1-N_i)^{1-s_i}$$

Proof:

$$N_i = \sum_{s \in S} s_i P(s)$$

$$1 - N_i = \sum_{s \in S} (1-s_i) P(s)$$

$$(*) = \sum_{i=0}^{r} \sum_{s \in S} \left(s_i P(s) \ln N_i + (1-s_i) P(s) \ln(1-N_i) \right)$$

$$= -\sum_{s\in S} P(s)\left(\sum_{j=0}^{5} s_i \ln(N_i) + (1-s_i)\ln(1-N_i)\right)$$

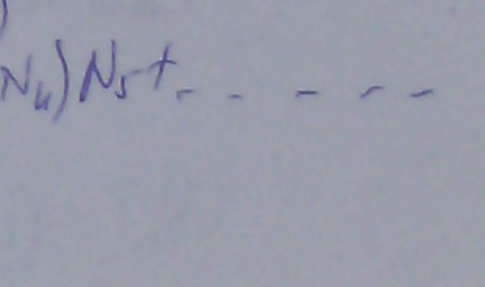
$$= \sum_{s\in S} P(s) \ln\left(\prod_{i=0}^{5} N_i^{s_i}(1-N_i)^{1-s_i}\right)$$

$$\Rightarrow \sum_{s\in S} P(s)\ln(P(s)) \overset{(*)}{\geq} \sum_{s\in S} P(s) \ln \prod_{j=0}^{5}\left(N_i^{s_i}(1-N_i)^{1-s_i}\right)$$

$$\Rightarrow \sum_{s\in S} P(s) \ln\left(\prod_{i=0}^{5} \frac{N_i^{s_i}(1-N_i)^{1-s_i}}{P(s)}\right) \leq 0$$

Note: Equality iff $P(s) = \prod_{i=0}^{5} N_i^{s_i}(1-N_i)^{1-s_i}$ $(*)$

otherwise using $\ln x < x-1 \quad (x\neq 1)$



$$\ln \prod_{i=0}^{5} \frac{N_i^{s_i}(1-N_i)^{1-s_i}}{P(s)} < \prod_{i=0}^{5} \frac{N_i^{s_i}(1-N_i)^{1-s_i}}{P(s)} - 1$$

$$\sum_{s\in S} P(s) \ln(\quad) \leq \left(\sum \prod_{i=0}^{5}(\quad) - P(s)\right)$$

($*$) doesn't hold

$$= \sum_{s\in S}\left(\prod_{i=0}^{5} N_i^{s_i}(1-N_i)^{1-s_i}\right) - 1$$

$P^{eq}(s)$

$$\sum_{s} N_0 N_1 N_2 N_3 N_4 N_5 + N_0 N_1 N_2 N_3 N_4 (1-N_5) + N_0 N_1 N_2 N_3 (1-N_4) N_5 + \cdots$$

$$= 1$$

rhs $= 0$

16/12 LGA: Equilibrium $N_i^{(eq)} = \dfrac{1}{1+e^{a+b\cdot c_i}}$ (Fermi-Dirac)

work out a, b as functions of

$$\rho = \sum_i N_i$$

$$\underline{u} = \frac{1}{\rho}\sum_i c_i N_i$$

$$N_i^{(eq)} = \rho\left(\frac{1}{6} + \frac{1}{3}\underbrace{c_{i\alpha}u_\alpha}_{c_i\cdot\underline{u}} + G(\rho)\underbrace{\Pi_{i\alpha\beta}u_\alpha u_\beta}_{(c_i\cdot\underline{u})^2 - \frac{1}{2}u^2}\right) \quad \text{(small velocity approximation)}$$

$$G(\rho) = \frac{1}{3}\frac{6-2\rho}{6-\rho} \qquad \Pi_{i\alpha\beta} = c_{i\alpha}c_{i\beta} - \frac{1}{2}\delta_{\alpha\beta}$$

problematic to reconcile consistency with NS

LGA to LBM

Step 1 Averaged LGA

$$N_i(r_i + c_i, t+1) = N_i(r,t) + C_i(N)$$

$$N = (N_i)_{i=0,1\cdots,5}$$

$$C_i(N) = \sum_{s s' \in S^2} (s_i' - s_i) \langle \xi_{s s'} \rangle \prod_{j=0}^{5} N_j^{s_j'} (1-N_j)^{1-s_j'}$$

Note: $C_i(N^{eq}) = 0$ $\quad \sum_i C_i = 0$

$$\sum_i c_i C_i = 0$$

Step 2 Linearize

$$N_i(r + c_i, t+1) = N_i(r,t) + \underbrace{\sum_{j=0}^{5} C_{ij}^{(0)} \left(N_j - N_j^{(eq)}\right)}_{C_i(N)}$$

Note: ~~$C(N_i^{eq})$~~

Can show $(1, \cdots, 1)$ $(c_{0\alpha}, \cdots, c_{5\alpha})$ are left eigenvectors of $C_{ij}^{(0)}$

Step 3 Model with enhanced collision

(a) in N_i^{eq} we set $G(s) = \frac{1}{3}\frac{6-2s}{6-s}$

$$f_i^{(eq)} = s\left\{\frac{1}{6} + \frac{1}{3} c_{i\alpha} u_\alpha + \frac{1}{3} s_{i\alpha\beta} u_\alpha u_\beta\right.$$

$$= s\left\{\frac{1}{6} + \frac{1}{3} G_{i\alpha} \cdot u - \frac{u^2}{6} + \frac{1}{3}(G_i \cdot u)^2\right\}$$

Consider MB. Distribution

$$f^{(MB)} = \frac{s}{(2\pi RT)^{1/2}} e^{-\frac{|c-u|^2}{2RT}}$$

$$= \underbrace{\frac{s}{2\pi RT} e^{-\frac{c^2}{2RT}}}_{A} \underbrace{e^{\frac{uc}{RT} - \frac{u^2}{2RT}}}_{(*)}$$

Note: $e^x = 1 + x + \frac{1}{2}x^2 + \cdots$

$$(*) = 1 + \frac{u\cdot c}{RT} - \frac{u^2}{2RT} + \frac{(c\cdot u)^2}{(RT)^2} + O(u^3)$$

$A = \frac{s}{6}$ $\quad RT = 1/2$ $\Rightarrow$ same as f_i

(b) Replace $C_{ij}^{(0)}$ with Matrix $A = (a_{ij})_{ij=1,\cdots 6}$ satisfying conservation

$$\sum_i c_i = 0 \qquad \sum_i c_i C_i = 0$$

$$C_i = \sum_j a_{ij}(f_j - f_j^{eq})$$

$a_{1,\alpha\beta}$ $\quad a_{2,\alpha\beta}$

Lattice Boltzmann Method

$A_{ij} = -\omega \delta_{ij}$ $\quad f(\underline{r}+\underline{c}_i, t+1) = f_i(\underline{r},t) + \underbrace{\frac{1}{\lambda}\left(f_i^{eq}(\underline{r},t) - f_i(\underline{r},t)\right)}_{C_i}$

$\rho := \sum f_i \overset{!}{=} \sum f_i^{eq}$

$\rho \underline{u} = \sum \underline{c}_i f_i \overset{!}{=} \sum \underline{c}_i f_i^{(eq)}$

$\Rightarrow C_i = f_i - f_i^{(eq)} = 0$

$\sum \underline{c}_i C_i = \sum_{i=0}^{b} \underline{c}_i \left(f_i - f_i^{(eq)}\right) = 0$

Remark: Algorithm

Set $f(\underline{r}, t=0)$ $\forall \underline{r}$

do $n = 1, 2, 3 \ldots$

- $\rho = \sum f_i$ $\quad \rho \underline{u} = \sum \underline{c}_i f_i$
- $f_i^{(eq)} = f_i^{(eq)}(\rho, \underline{u})$
- $f_i' = \omega (f_i^{(eq)} - f_i)$ } local collision
- $f(\underline{r}+\underline{c}_i, t+1) = f_i(\underline{r},t) + f_i'$ } streaming
- Boundary conditions

end do

$$f_i^{eq} = \rho w_i \left(1 + \frac{\underline{c}_i \cdot \underline{u}}{c_s^2} - \frac{\underline{u}^2}{2c_s^2} + \frac{1}{2}\frac{(\underline{c}_i \cdot \underline{u})^2}{c_s^4}\right) \qquad c_s^2 = RT$$

Computation of w_i

Review: Quadrature

$$I(f) = \int_a^b f \, dx \approx \sum_{i=1}^{n} \alpha_i f(x_i) = I_n(f)$$

(α_i: weights, x_i: nodes)

Def^n: (degree of precision d.o.p.)

We say $I_n(f)$ has dop $m \in \mathbb{N}$

if $I(x^l) - I_n(x^l) = 0 \quad \forall\, l \le m$ $\quad l = 0, \ldots, m$

optimal quadrature rule: Gaussian $\quad m = 2n-1$

Weighted Integrals

$$I^{(\omega)}(f) = \int_a^b \underbrace{\omega(x)}_{>0} f(x) \, dx = \sum_{i=1}^{n} \alpha_i f(x_i) = I_n^{(\omega)}(f)$$

Still: $I^{(\omega)}(x^l) - I_n^{(\omega)}(x^l) = 0 \qquad l = 0, \ldots, 2n-1$

for Gaussian rule

Example: $w(x) = e^{-x^2}$ $\quad a = -\infty$, $b = \infty$

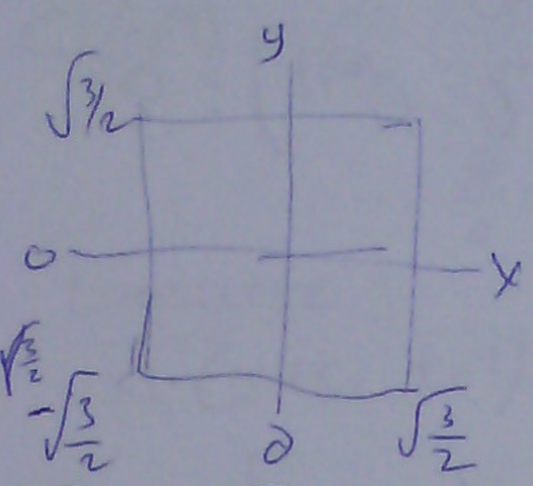
$\Rightarrow$ Gauss Hermite quadrature

Multivariate case

$$I^{(w)}(f) = \int_{\mathbb{R}^2} e^{-(x^2+y^2)} f(x,y)\,dx\,dy \approx \sum_{i,j=1}^{n} \alpha_i \beta_j f(x_i, y_j)$$

(x^2+y^2; $\alpha_i\beta_j$: same as 1D)

eg.



$\alpha_i = \frac{\sqrt{\pi}}{6}, \frac{2\sqrt{\pi}}{3}, \frac{\sqrt{\pi}}{6}$

Recall: $\overset{MB}{=}$

$$\tilde{f}^{(eq)} = \frac{\rho}{2\pi RT} e^{-\frac{c^2}{2RT}} \left\{ 1 + \frac{\underline{c}\cdot\underline{u}}{RT} - \frac{u^2}{2RT} + \frac{1}{2}\frac{(\underline{c}\cdot\underline{u})^2}{(RT)^2} \right\} \quad (*)$$

$$\int_{\mathbb{R}^2} \tilde{f}^{(eq)}\,d\underline{c} = \rho \qquad \int_{\mathbb{R}^2} \tilde{f}^{(eq)} \underline{c}\,d\underline{c} = \rho\underline{u}$$

Want: $\sum_{i=0}^{?} f_i^{(eq)} = \rho \qquad \sum c_i f_i^{(eq)} = \rho\underline{u}$

& possibly higher order moments (same as from MB)

Consider:

$$I = \int_{\mathbb{R}^2} \tilde{f}^{(eq)} c_1^n c_2^m\,d\underline{c} \quad \text{of } f^{(eq)} \text{ as in } (*)$$

↑ Replace with Gauss-Hermite quadrature

22/12 **Multiscale Expansion**

Consider ODE

(i) $y'' + y = 0 \qquad y(0) = 0 \qquad y'(0) = 1$

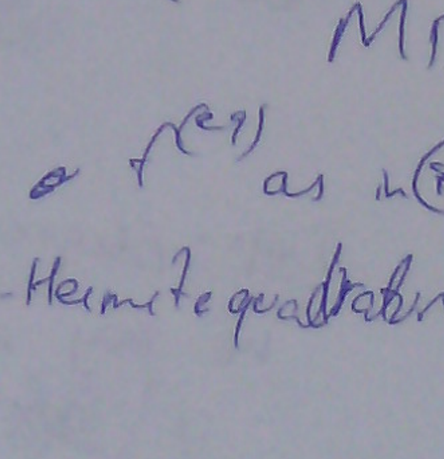
$y(t) = \sin t$

Relevant time scale $T = 2\pi \sim O(1)$

(ii) $y' + \varepsilon y = 0 \qquad y(0) = 1$

$y(t) = a e^{-\varepsilon t}$

$y(t) = e^{-\varepsilon t}$

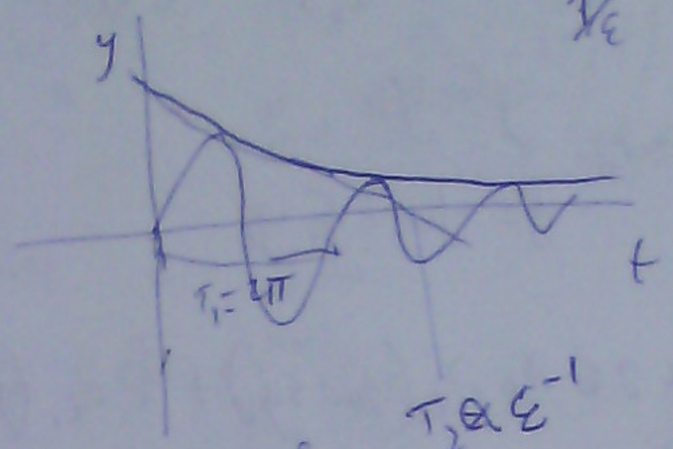


$T = 1/\varepsilon \qquad (\varepsilon \ll 1)$

(iii) $y'' + \varepsilon y' + y = 0 \qquad y(0) = 0 \quad y'(0) = 1 \qquad \varepsilon \ll 1$

$$y(t) = \frac{1}{\sqrt{1-\varepsilon^2/4}} e^{-\frac{\varepsilon}{2}t} \sin\left(t\sqrt{1-\frac{\varepsilon^2}{4}}\right)$$

$\frac{1}{\varepsilon}$ $\qquad \approx 1$



~~Perturbation analysis~~

Perturbation analysis

$$y(t) = \sum_{k=0}^{\infty} y_k(t)\varepsilon^k = y_0(t) + \varepsilon y_1(t) + O(\varepsilon^2)$$

substitute into ODE (iii) (neglect $O(\varepsilon^2)$ terms)

$$y_0'' + \varepsilon y_1'' + \varepsilon(y_0' + \varepsilon y_1') + y_0 + \varepsilon y_1 = 0$$

$$y_0(0) + \varepsilon y_1(0) = 0$$
$$y_0'(0) + \varepsilon y_1'(0) = 1$$

$$y_0'' + y_0 + \varepsilon(y_1'' + y_0' + y_1) + \varepsilon^2 y_1' = 0$$

ε^0	$y_0'' + y_0 = 0$	$y_0 = 0$	$y_0'(0) = 1$	$y_0(t) = \sin t$
ε^1	$y_1'' + y_0' + y_1 = 0$ $y_1'' + y_1 = -\cos(t)$	$y_1(0) = 0$	$y_1'(0) = 0$	$y_1(t) = \frac{1}{2} t \sin t$

$$y(t) = \sin(t) + \frac{1}{2}\varepsilon t \sin t$$

$|y(t)| \to \infty \qquad t \to \infty$

Multiscale (Two-scale)

Explicitly let y be func. of two time scales

$$y(t) = \sum y_k(t_1(t), t_2(t))\varepsilon^k$$

$$t_1 = t \qquad t_2 = \varepsilon t$$

$$y' = \frac{\partial y}{\partial t_1}\frac{\partial t_1}{\partial t} + \frac{\partial y}{\partial t_2}\frac{\partial t_2}{\partial t} = \frac{\partial y}{\partial t_1} + \varepsilon\frac{\partial y}{\partial t_2}$$

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Substitute into ODE

$$\partial_t(\partial_{t_1} y + \varepsilon \partial_{t_2} y) + \varepsilon(\partial_{t_1} y + \varepsilon \partial_{t_2} y) + y = 0$$

$$\partial_{t_1}^2 y + 2\varepsilon \partial_{t_1}\partial_{t_2} y + \varepsilon^2 \partial_{t_2}^2 y + \varepsilon(\partial_{t_1} y + \varepsilon \partial_{t_2} y) + y = 0$$

~~$\partial_t(y) + y = 0$~~ ~~$y = y_0$~~

$$y = y_0 + \varepsilon y_1$$

$$\partial_{t_1}^2(y_0 + \varepsilon y_1) + 2\varepsilon \partial_{t_1}\partial_{t_2}(y_0 + \varepsilon y_1) + \varepsilon \partial_{t_1}(y_0 + \varepsilon y_1) + (y_0 + \varepsilon y_1) = 0$$

$y_0 + \varepsilon y_1 \neq 0$ ~~$= 0$~~

$\partial_{t_1}(y_0 + \varepsilon y_1) + \varepsilon \partial_{t_2}(y_0 + \varepsilon y_1) \neq 1$

ε^0: $\partial_{t_1}^2 y_0 + y_0 = 0$ $\quad y_0 = 0$ $\quad \partial_{t_1} y_0 = 1$ ~~$y_0(t) = \sin(t_1)$~~

$y_0(t) = a(t_2)\sin(t_1) + b(t_2)\cos(t_1)$

$b_0(0) = 0$ (1)

$a_0(0) = 1$ (2)

ε^1: $\partial_{t_1}^2 y_1 + 2\partial_{t_1}\partial_{t_2} y_0 + \partial_{t_1} y_0 + y_1 = 0$

$\partial_{t_1}^2 y_1 + y_1 = -2\partial_{t_1}\partial_{t_2} y_0 - \partial_t y_0$

$\partial_{t_1}^2 y_1 + y_1 = -2(a_0'(t_2)\cos t_1 + b_0'(t_2)\sin t_1)$

$\quad - a_0(t_2)\cos t_1 + b_0(t_2)\sin t_1$

$\partial_{t_1}^2 y_1 + y_1 = -(2a_0' + a_0)\cos t_1 + (2b_0' + b_0)\sin t_1$

Kill growth terms $= 0$ $\quad a_0 = e^{-\frac{1}{2}t_2}$ $\quad = 0$ $\quad b_0 = 0 e^{-t_2/2} = 0$

$y_0(t) = e^{-t_2/2}\sin t_1 = e^{-\varepsilon t/2}\sin t$

23/12

Previously:

Linearized (averaged) LGA.

$$N_i(\underline{r} + \underline{c}_i, t+1) = N_i(\underline{r}, t) + C_{ij}^{(0)}\left(N_j(\underline{r}, t) - N_j^{(eq)}\right)$$

collision operator of averaged LGA: $\left.\frac{\partial C_i(N)}{\partial N_j}\right|_{u=0}$ $\quad C^{lin}(N)$

Conservation:

$$C_i^{lin}(N^{(eq)}) = 0$$

$$\sum_i C_i^{(lin)} = 0 \qquad \sum_i \underline{c}_i C_i^{lin} = 0$$

$$f_i(\underline{r} + \underline{c}_i, t+1) = f_i(\underline{r}, t) + \omega\left(f_i^{eq}(\underline{r}, t) - f_i(\underline{r}, t)\right)$$

$C_{ij} = -\omega \delta_{ij}$ $\quad C_i$

moments $\quad a_{1,\alpha\beta}^{(1)} \quad \cdots \quad a_{2,\alpha\beta}^{(1)}$

$$f_i^{(eq)} = \rho w_i \left(1 + \frac{c_i \cdot u}{c_s^2} - \frac{u^2}{2c_s^2} + \frac{1}{2}\frac{(c_i \cdot u)^2}{(RT)^2}\right)$$

$$c_s^2 = RT$$

Note: $\rho = \sum_i f_i(r,t)$

$$\rho u = \sum_i c_i f_i$$

Determine w_i s.th $c_i = (c_{i,1}; c_{i,2})^T$

$$\sum_i f_i^{(eq)} c_{i,1}^m c_{i,2}^n = \int_{\mathbb{R}^2} \tilde{f}^{(eq)} c_1^m c_2^n \, dc_1 dc_2 \quad \text{up to some degree } m, n \geq 1$$

$$\tilde{f}^{(eq)} = \frac{\rho}{2\pi RT} e^{\frac{-c^2}{2RT}} \left(1 + \frac{c \cdot u}{RT} - \frac{u^2}{RT} + \frac{1}{2}\frac{(c \cdot u)^2}{(RT)^2}\right)$$

know: $\int_{\mathbb{R}^2} \tilde{f}^{(eq)} dc = \rho \qquad \int_{\mathbb{R}^2} \tilde{f}^{(eq)} c \, dc = \rho u$

In particular, then we have

$$\sum_i f_i^{eq} = \rho = \sum_i f_i \Rightarrow \sum_i c_i = 0$$

$$\sum_i c_i f_i^{eq} = \rho u = \sum_i f_i c_i \Rightarrow \sum_i c_i C_i = 0$$

Recall: Gauss-Hermite Quadrature

$$\int_{\mathbb{R}} e^{-x^2} g(x) = \sum_{i=1}^{\lambda} w_i \, g(x_i) + R_m$$

Set $c = \sqrt{2RT}\,\xi$

Then $I = \int_{\mathbb{R}^2} \tilde{f}^{(eq)} c_1^m c_2^n \, dc_1 dc_2$

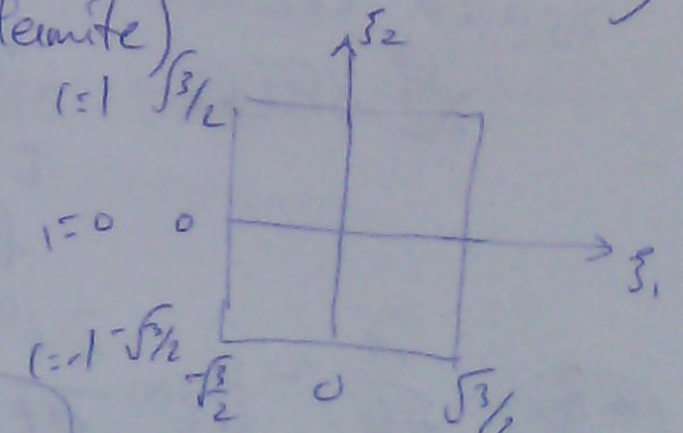
$$= \frac{\rho}{\pi} (2RT)^{\frac{m+n}{2}} \int_{\mathbb{R}^2} \xi_1^m \xi_2^n e^{-\xi^2} \left(1 + \frac{\sqrt{2}\,\xi \cdot u}{\sqrt{RT}} - \frac{u^2}{2RT} + \frac{(\xi \cdot u)^2}{RT}\right) d\xi_1 d\xi_2$$

Use 3-point Rule: (Gauss-Hermite)

$$\sum_{i=1}$$

$$\omega_{-1} = \omega_1 = \sqrt{\pi}/6$$

$$\omega_0 = \frac{2\sqrt{\pi}}{3}$$



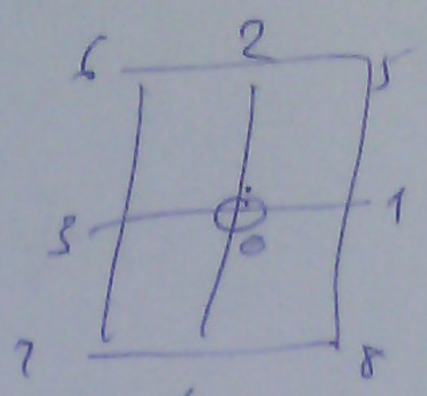
$$\Rightarrow I \approx \rho (2RT)^{\frac{m+n}{2}} \sum_{k,l=-1}^{1} \frac{\omega_k \omega_l}{\pi} \xi_{1k}^m \xi_{2l}^n \left(1 + \sqrt{2}\frac{\xi_{1k} u_1 + \xi_{2l} u_2}{\sqrt{RT}} - \frac{u_1^2 + u_2^2}{2RT} + \frac{(\xi_{1k} u_1 + \xi_{2l} u_2)^2}{RT}\right)$$

(ω_i: ω_1)

Note: $\xi_{1k} u_1 + \xi_{2l} u_2 = \sqrt{\frac{3}{2}}(k u_1 + l u_2)$

$= \sqrt{\frac{3}{2}} \left(\tilde{\underline{\underline{C}}}_{k,l} \cdot \underline{\underline{\Pi}} \right)$ $\qquad \tilde{\underline{\underline{C}}}_{k,l} = (k,l)^T$

$$\frac{\omega_k \omega_l}{\pi} = \begin{cases} 4/9 & k=l=0 \\ 1/9 & k=0, l\neq 0 \\ & l=0, k\neq 0 \\ 1/36 & |k|=|l|=1 \end{cases}$$



Set $\tilde{u} = u/\sqrt{2RT}$

$$f_i^{(eq)} = \begin{cases} 4/9\, \rho \left\{ 1 - \frac{3}{2} u^2 \right\} & i=0 \\ 1/9\, \rho \left(1 + 3\tilde{\underline{C}}_i \cdot \tilde{\underline{u}}_i + \frac{9}{2} (\tilde{\underline{C}}_i \cdot \tilde{\underline{u}})^2 - \frac{3}{2} (\tilde{u})^2 \right) & i=1,2,3,4 \\ \frac{1}{36} \rho \{ \quad \downarrow \quad \} & i=5,6,7,8 \end{cases}$$

Multiscale expansion

Recall: LBM (D2Q9)

(1) $f_i(\underline{r} + \underline{c}_i, t+1) = f_i(\underline{r}, t) + \omega \left(f_i(\underline{r}, t) + f_i^{eq}(\underline{r}, t) \right)$

(2) $\sum_{i=0}^{8} f_i^{(eq)} = \sum_{i=0}^{8} f_i = \rho$

(3) $\sum_{i=0}^{8} \underline{c}_i \underline{f}_i^{eq} = \sum_{i=0}^{8} \underline{c}_i f_i = \rho u$

Relevant scales: (spatial $\ll$ temporal) (ref $\varepsilon = 1/N$

- (1) Lattice 'Knudsen' number $= \frac{\Delta x}{L} = \mathcal{O}(\varepsilon) = \mathcal{O}\left(\frac{1}{N}\right)$ (N: #nodes/dim; $L = 1$)

- (2) (i) convective scale $\mathcal{O}(N)$
  (ii) diffusive scale $\mathcal{O}(N^2)$

Scaled coordinates:

$r_\alpha^{(1)} = \varepsilon r_\alpha$

$t^{(1)} = \varepsilon t$

$t^{(2)} = \varepsilon^2 t$

(**) $\frac{\partial}{\partial t} = \frac{\partial}{\partial t^{(1)}} \frac{\partial t^{(1)}}{\partial t} + \frac{\partial}{\partial t^{(2)}} \frac{\partial t^{(2)}}{\partial t} = \varepsilon \partial_t^{(1)} + \varepsilon^2 \partial_t^{(2)}$

$\frac{\partial}{\partial r_\alpha} = \varepsilon \partial_\alpha^{(1)}$

Need to expand:

$$f_i = \sum_{k=0}^{\infty} \varepsilon^k f_i^{(k)} = \sum_{0}^{\infty} \varepsilon^k f^{(k)}\left(r^{(1)}(r), t^{(1)}(t), t^{(2)}(t)\right)$$

(***) $$f_i = f_i^{(0)} + \varepsilon f_i^{(1)} + \mathcal{O}(\varepsilon^2)$$ 9

(*) $$f_i(r + \underbrace{c_i \Delta t}_{\Delta r_\alpha}, t + \Delta t) \approx f_i(r,t) + \partial_{r_\alpha} f_i \underbrace{c_{i\alpha} \Delta t}_{\Delta r_\alpha} + \partial_t f_i \Delta t$$
$$+ \frac{1}{2}\Delta t^2 \left(\partial_t \partial_t f_i + 2 c_{i\alpha} \partial_{r_\alpha} \partial_t f_i + c_{i\alpha} c_{i\beta} \partial_{r_\alpha} \partial_{r_\beta} f_i\right)$$

no summation over i

Substitute (*) in (1)

$$\Rightarrow \partial_{r_\alpha} f_i c_{i\alpha} \Delta t + \partial_t f_i \Delta t + \frac{1}{2}(\Delta t)^2 (\ldots) - \omega\left(f_i(r,t) - f_i^{(eq)}(r,t)\right) = 0$$

Substitute (**), (***) into ↑

$$E_i^{(0)} + \varepsilon E_i^{(1)} + \varepsilon^2 E_i^{(2)} \ldots = 0$$

$E_i^{(n)}$ contains only terms $\partial_t^{(k)} f_i^{(l)}$ with $k+l = n$

$E_i^{(0)} = 0$ if $f_i^{(0)} = f_i^{(eq)}$

$$E_i^{(1)} = c_{i\alpha} \partial_\alpha^{(1)} f_i^{(0)} \Delta t + \partial_t^{(1)} f_i^{(0)} \Delta t + \omega f_i^{(1)}$$

$$E_i^{(2)} = c_{i\alpha} \Delta t\, \partial_\alpha^{(1)} f_i^{(1)} + \Delta t\, \partial_t^{(1)} f_i^{(1)} + \Delta t\, \partial_t^{(2)} f^{(0)} + \frac{\Delta t^2}{2}\left(\partial_t^{(1)} \partial_t^{(1)} f_i^{(0)} + 2 c_{i\alpha} \partial_\alpha^{(1)} \partial_t^{(1)} f_i^{(0)} + c_{i\alpha} c_{i\beta} \partial_\alpha^{(1)} \partial_\beta^{(1)} f_i^{(0)}\right) + \omega f_i^{(2)} = 0$$

Moments

(A) $= \sum_i E_i^{(1)}$

(B) $= \sum_i c_i E_i^{(1)}$

(C) $= \sum_i E_i^{(2)}$

(D) $= \sum_i c_i E_i^{(2)}$

Claim

(A) + ε(B) = 0

(C) + ε(D) = 0

Consistent with Navier-Stokes.

$+ 2\rho c_\alpha \partial_\beta^{(1)} (\rho u_\beta)$

$\partial_t^{(1)} \Sigma_\alpha^{(1)} (\rho u_\alpha) + 3 \partial_\alpha^{(1)} \partial_\beta^{(1)} (\rho u_\beta)$

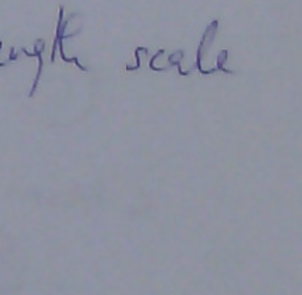
2011

Multiscale Expansion

LBM

(1) $f_i(r + c_i \Delta t, t + \Delta t) = f_i(r,t) + \omega (f_i^{eq}(r,t) - f_i(r,t)) \quad i = 0, 1 \cdots 8$

$$f_i^{(eq)} = \rho w_i \left\{ 1 + 3(c_i \cdot u) - \frac{3}{2} u^2 + \frac{9}{2} (c \cdot u)^2 \right\}$$



(2) $\sum_{i=0}^{8} f_i(r,t) = \sum_{i=0}^{8} f_i^{(eq)}(r,t) = \rho$

(3) $\sum_{i=0}^{8} c_i f_i(r,t) = \sum_{i=0}^{8} c_i f_i^{(eq)}(r,t) = \rho u$

Relevant spatial & temporal scales

Let $\varepsilon = \frac{1}{N}$

* 'Lattice Knudsen' number $\frac{\Delta x}{L} = O(N^{-1}) = O(\varepsilon)$ ← characteristic length scale

* (i) convective time scale $O(N)$

(ii) diffusive time scale $O(N^2)$

Introduce scaled coordinates

$r^{(1)} = \varepsilon r \qquad r = N \Rightarrow r^{(1)} = 1$

$t^{(1)} = \varepsilon t \qquad t = N \Rightarrow t^{(1)} = 1$

$t^{(2)} = \varepsilon^2 t \qquad t = N^2 \Rightarrow t^{(2)} = 1$

We will set $f_i = \sum_{k=0}^{\infty} \varepsilon^k f_i^{(k)}$

$f_i^{(k)} = f_i^{(k)}(r^{(1)}, t^{(1)}(t), t^{(2)}(t))$

$\frac{\partial}{\partial t} = \underbrace{\frac{\partial t^{(1)}}{\partial t}}_{\varepsilon} \frac{\partial}{\partial t^{(1)}} + \underbrace{\frac{\partial t^{(2)}}{\partial t}}_{\varepsilon^2} \frac{\partial}{\partial t^{(2)}}$

Notation $\partial_t = \varepsilon \partial_t^{(1)} + \varepsilon^2 \partial_t^{(2)}$ → (4)

$\frac{\partial}{\partial r} = \varepsilon \frac{\partial}{\partial r^{(1)}} \rightarrow \partial_{r_\alpha} = \varepsilon \partial_{r_\alpha}^{(1)}$

$f_i = f_i^{(0)} + \varepsilon f_i^{(1)} + \varepsilon^2 f_i^{(2)} + \cdots$ (5)

Note: $\sum_i f_i^{(k)(1)} = 0 \qquad \sum_i c_i f_i^{(k)(1)} = 0 \qquad k \geq 1 \quad (f^0 = f^{eq})$

not summed over i

(6) $f_i(r + c_i \Delta t, t + \Delta t) = f_i(r,t) + c_{i,\alpha} \Delta t \, \partial_\alpha f_i + \partial_t f_i \Delta t + \frac{\Delta t^2}{2} \{ \partial_t \partial_t f_i + 2 c_{i,\alpha} \partial_\alpha \partial_t f_i + c_{i,\alpha} c_{i,\beta} \partial_\alpha \partial_\beta f_i \} + O(\Delta t)^3$

Subst

Substitute ⑥ into ①

$$c_{i\alpha}\Delta t\,\partial_\alpha f_i + \Delta t\,\partial_t f_i + \frac{\Delta t^2}{2}\{\dots\} - \omega(f^{(eq)} - f_i) \approx 0 \quad ⑦$$

Substitute (4), (5) into ⑦

⑦ $\Rightarrow$ $E_i^{(0)} + \varepsilon E_i^{(1)} + \varepsilon^2 E_i^{(2)} + \dots$

where each $E^{(k)}$ contains terms like

$\partial_t^{(l)} f^{(m)}$ s.t. $l+m=k$

$$E_i^{(0)} = f^{(0)} = f^{(eq)}$$

$$E_i^{(1)} = c_{i\alpha}\Delta t\,\partial_\alpha^{(1)} f_i^{(0)} + \Delta t\,\partial_t^{(1)} f_i^{(0)} + \omega f_i^{(1)}$$

$$E_i^{(2)} = \Delta t\,\partial_t^{(1)} f_i^{(1)} + \Delta t\,\partial_t^{(2)} f_i^{(0)} + c_{i\alpha}\Delta t\,\partial_\alpha^{(1)} f^{(1)} + \frac{(\Delta t)^2}{2}\{\partial_t^{(1)}\partial_t^{(1)} f_i^{(0)} + 2c_{i\alpha}\partial_\alpha^{(1)}\partial_t^{(1)} f_i^{(0)} + c_{i\alpha}c_{i\beta}\partial_\alpha^{(1)}\partial_\beta^{(1)} f_i^{(0)}\} + \omega f^{(2)}$$

Moments:

Ⓐ $\sum_{i=0}^{8} E_i^{(1)}$ Ⓑ $\sum c_i E_i^{(1)}$

Ⓒ $\sum E_i^{(2)}$ Ⓓ $\sum c_i E_i^{(2)}$

Claim

$$\sum E_i^{(1)} + \varepsilon_0 E_i^{(2)} = 0$$

$$\sum c_i (E^{(1)} + \varepsilon E_i^{(2)}) = 0 \quad \text{gives 'NSE'}$$

Ⓐ $\frac{1}{\Delta t}\sum_i E_i^{(1)} = \sum_i (\partial_t^{(1)} f_i^{(0)} + c_{i\alpha}\partial_\alpha^{(1)} f_i^{(0)} + \frac{\omega}{\Delta t} f_i^{(1)}) \to 0$ (2)

$= \partial_t^{(1)} \underbrace{\sum f_i^{(0)}}_{\rho} + \partial_\alpha^{(1)} \underbrace{\sum_i c_{i\alpha} f_i^{(0)}}_{\rho u_\alpha}$

$= \partial_t^{(1)} \rho + \partial_\alpha^{(1)} (\rho u_\alpha)$

Ⓑ $\frac{1}{\Delta t}\sum_i c_{i\alpha} E_i^{(1)} = \sum_i c_{i\alpha}\partial_t^{(1)} f_i^{(0)} + \sum_i c_{i\alpha}c_{i\beta}\partial_\beta^{(1)} f_i^{(0)} + \frac{\omega}{\Delta t}\sum_i f_i^{(1)} c_{i\alpha}$ $\to 0$ (3)

$= \partial_t^{(1)}\underbrace{(\sum_i c_{i\alpha} f_i^{(0)})}_{\rho u_\alpha} + \partial_\beta^{(1)}\underbrace{(\sum_i c_{i\alpha}c_{i\beta} f_i^{(0)})}_{P_{\alpha\beta}^{(0)}}$

Ⓒ $\frac{1}{\Delta t}\sum_i E_i^{(2)} = \partial_t^{(2)}\rho + \frac{\Delta t}{2}\{\partial_t^{(1)}\partial_t^{(1)}\rho + 2\partial_\alpha^{(1)}\partial_t^{(1)}\rho u_\alpha + \partial_\alpha^{(1)}\partial_\beta^{(1)} P_{\alpha\beta}^{(0)}\} + \frac{\omega}{\Delta t}\sum_i f_i^{(2)} \to 0$

$= \partial_t^{(2)}\rho + \frac{\Delta t}{2}\Big[\underbrace{\partial_t^{(1)}(\partial_t^{(1)}\rho + \partial_\alpha^{(1)}\rho u_\alpha)}_{\alpha(\varepsilon)} + \partial_\alpha^{(1)}\partial_\beta^{(1)}\rho u_\alpha u_\beta + \partial_\alpha^{(1)}\partial_\beta^{(1)} P_{\alpha\beta}^{(1)}\Big]$

$= \partial_t^{(2)}\rho + \frac{\Delta t}{2}\partial_\alpha^{(1)}\{\underbrace{\partial_t^{(1)}\rho u_\alpha + \partial_\beta^{(1)} P_{\alpha\beta}}_{\alpha(\varepsilon)}\}$

$$\frac{\varepsilon}{\Delta t}\sum E^{(1)} + \frac{\varepsilon^2}{\Delta t}\sum E_i^{(2)} = \varepsilon\,\partial_t^{(1)}\rho + \varepsilon^2\partial_t^{(2)}\rho + \varepsilon\partial_\alpha^{(1)}(\rho u_\alpha)$$

$$= \boxed{\partial_t(\rho) + \partial_\alpha(\rho u_\alpha) = 0}$$

$\partial_t^{(2)}(\rho u_\alpha) - \Delta t$ ($= \omega$ / ... $+ 2(\partial_\alpha^{(1)} \partial_\beta^{(1)}(\rho u_\beta))$

$\cdots \partial_\alpha^{(1)} \partial_\alpha^{(1)}(\rho u_\alpha) + 3\,\partial_\alpha^{(1)} \partial_\beta^{(1)}(\rho u_\beta)$

Need to finish moment (B)

$$(B) = \frac{1}{\Delta t}\sum c_{i\alpha} E_i^{(1)} = \partial_t^{(1)} \rho u_\alpha + \partial_\beta^{(1)}\left(c_{i\alpha} c_{i\beta} f_i^{(0)}\right)$$

$$P_{\alpha\beta}^{(0)} = \sum c_{i\alpha} c_{i\beta} \rho w_i \left\{1 + 3(c_i \cdot u) - \frac{3u^2}{2} + \frac{9}{2}(c_i \cdot u)^2\right\}$$

$P_{\alpha\beta}^{(0)}$

$$= P_{\alpha\beta}^{(0,1)} + P_{\alpha\beta}^{(0,2)} + P_{\alpha\beta}^{(0,3)} + P_{\alpha\beta}^{(0,4)}$$

$$P_{\alpha\beta}^{(0,1)} = \rho \sum_i w_i c_{i\alpha} c_{i\beta} \qquad w_0 = \frac{4}{9}\quad w_i = \frac{1}{9}\ i = 1,2,3,4$$

$$w_i = \frac{1}{36}\ i = 5,6,7,8$$

eg. $\alpha = \beta = 1$ $\qquad \sum w_i c_{i1}{}^2 = \frac{1}{9} + 4\cdot\frac{1}{36} = \frac{1}{3}$

$$P_{\alpha\beta}^{(0,1)} = \frac{\rho}{3}\delta_{\alpha\beta}$$

Recall: $c_i^* \alpha = c_0^* (c_s^*)^2 = RT^*$

dimensionless

$$\left(\frac{c_0^*}{c_s^*}\right)^2 = 3$$

$$\Rightarrow \frac{1}{3} = \left(\frac{c_s^*}{c_0^*}\right)^2 = \frac{RT^*}{c_0^*} \qquad S = \frac{\rho^*}{\rho_{ref}}$$

$$P_{\alpha\beta}^{(0,1)} = \frac{\rho^*}{\rho_{ref}} \frac{RT^*}{c_0^*} \delta_{\alpha\beta} = \frac{P^* \delta_{\alpha\beta}}{\rho_{ref}(c_0^*)^2} = P\delta_{\alpha\beta}$$

Also $\quad P_{\alpha\beta}^{(0,2)} = 3\rho u_\gamma \sum w_i c_{i\alpha} c_{i\beta} c_{i\gamma} = 0$

$$P_{\alpha\beta}^{(0,3)} = -\frac{3}{2}(u_1^2 + u_2^2)\rho \underbrace{\sum w_i c_{i\alpha} c_{i\beta}}_{\frac{1}{3}\delta_{\alpha\beta}} = -\frac{1}{2}(u_1^2 + u_2^2)\rho\delta_{\alpha\beta}$$

$$P_{\alpha\beta}^{(0,4)} = \frac{9}{2}\rho \sum_i w_i c_{i\alpha} c_{i\beta} \underbrace{(c_i \cdot u)^2}_{u_1^2 c_{i1}^2 + 2c_{i1}c_{i2}u_1 u_2 + c_{i2}^2 u_2^2}$$

$$P_{\alpha\beta}^{(0,4)} = \begin{cases} \frac{3}{2}\rho u_1^2 + \frac{1}{2}\rho u_2^2 & \alpha = \beta = 1 \\ \rho u_\alpha u_\beta & \alpha \neq \beta \\ \frac{1}{2}\rho u_1^2 + \frac{3}{2}\rho u_2^2 & \alpha = \beta = 2 \end{cases}$$

$$P_{11}^{(0)} = P - \frac{1}{2}(u_1^2 + u_2^2)\rho + \frac{3}{2}\rho u_1^2 + \frac{1}{2}\rho u_2^2 = P + \rho u_1^2$$

Similarly $P_{22}^{(0)} = P + \rho u_2^2$

$$P_{\alpha\beta}^{(0)} = \rho u_\alpha u_\beta \quad (\alpha \neq \beta)$$

$$P_{\alpha\beta}^{(0)} = P\delta_{\alpha\beta} + \rho u_\alpha u_\beta$$

$$\frac{1}{\Delta t}\sum c_{i\alpha} E_i^{(1)} = \partial_t^{(1)}(\rho u_\alpha) + \partial_\beta^{(1)} P_{\alpha\beta}^{(0)}$$

$$= \partial_t^{(1)}(\rho u_\alpha) + \partial_\alpha^{(1)} P + \partial_\beta^{(1)}(\rho u_\alpha u_\beta)$$

Substitute ⑥ into ①

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$$\varepsilon A + \varepsilon^2 B = 0 \Rightarrow \quad \partial_t(\rho u_\alpha) + \partial_\beta(\rho u_\alpha u_\beta)$$

$$\varepsilon C + \varepsilon^2 D = 0$$

↓ todays

$$\partial_t^{(1)}(\rho u_\alpha) + \partial_\beta^{(1)}(\rho u_\alpha u_\beta) + \partial_\alpha p$$

$$\frac{1}{\Delta t} E_i^{(0)} = \partial_t^{(1)} f_i^{(1)} + \partial_t^{(2)} f_i^{(0)} + c_{i\alpha}\partial_\alpha^{(1)} f^{(1)} + \frac{1}{2}\Delta t\Big(\partial_t^{(1)}\partial_t^{(1)} f_i^{(0)} + 2 c_{i,\alpha}\partial_t^{(1)}\partial_\alpha^{(1)} f_i^{(0)}$$

($\partial_t^{(1)} f_i^{(1)}$ → 0)

$$+ c_{i\beta} c_{i\alpha}\partial_\alpha^{(1)}\partial_\beta^{(1)} f_i^{(0)} + \frac{\omega}{\Delta t} f_i^{(0)}$$

$$\Rightarrow \frac{1}{\Delta t} c_{i\alpha} E_i^{(2)} = \partial_t^{(1)}(\rho u_\alpha) + \partial_\beta^{(1)} \sum c_{i\alpha} c_{i\beta} f_i^{(1)} + \frac{1}{2}\Delta t\Big(\partial_t^{(1)}\partial_t^{(1)}(\rho u_\alpha) + 2\partial_t^{(1)}\partial_\beta^{(1)} P_{\alpha\beta}$$

$$+ \underbrace{\partial_\beta^{(1)}\partial_\gamma^{(1)} \sum_i c_{i\alpha} c_{i\beta} c_{ij} f_i^{(0)}}_{(**)}$$

$$\frac{1}{\Delta t} E^{(0)} = \partial_t^{(1)} f_i^{(0)} + c_{i\alpha}\partial_\alpha^{(1)} f_i^{(0)} + \frac{\nu}{\Delta t} f_i^{(0)} \quad (*)$$

finally $\varepsilon \to 0$ in $\varepsilon A + \varepsilon^2 B = 0$

$$f_i^{(1)} = -\frac{\Delta t}{\omega}\left\{\partial_t^{(1)} f_i^{(0)} + c_{i\alpha}\partial_\alpha^{(1)} f_i^{(0)}\right\}$$

$$\Rightarrow \frac{1}{\Delta t}\sum_i c_{i\alpha} E_i^{(0)} = \partial_t^{(2)}(\rho u_\alpha) - \frac{\Delta t}{\omega}\partial_\beta^{(1)}\partial_t^{(1)} \underbrace{\sum c_{i\alpha} c_{i\beta} f_i^{(0)}}_{P_{\alpha\beta}} - \frac{\Delta t}{\omega}\partial_\beta^{(1)}\partial_\gamma^{(1)} \sum_i c_{i\alpha} c_{i\beta} c_{i\gamma} f_i^{(0)}$$

$$+ \frac{1}{2}\Delta t \{(**)\}$$

$$\Rightarrow \partial_t^{(0)}(\rho u_\alpha) + \Delta t\left(1 - \frac{1}{2\omega}\right)\partial_t^{(1)}\partial_\beta^{(1)} P_{\alpha\beta} + \frac{1}{\Delta t}\left(\frac{1}{2} - \frac{1}{\omega}\right)\partial_\alpha^{(1)}\partial_\gamma^{(1)} \sum_i c_{i\alpha} c_{i\beta} c_{i\gamma} f_i^{(0)}$$

$$+ \frac{1}{2}\Delta t\, \partial_t^{(1)}\partial_t^{(1)}(\rho u_\alpha)$$

disappears ε

Recall: momentum

$$\partial_t(\rho u_\alpha) + \underbrace{\partial_\beta(\rho u_\alpha u_\beta)}_{\partial_\beta P_{\alpha\beta}} + \partial_\alpha p = O(\varepsilon)$$

$$= \partial_t^{(0)}(\rho u_\alpha) + \Delta t\left(\frac{1}{2} - \frac{1}{\omega}\right)\partial_t^{(1)}\partial_\beta^{(1)} P_{\alpha\beta} + \Delta t\left(\frac{1}{2} - \frac{1}{\omega}\right)\partial_\beta^{(1)}\partial_\gamma^{(1)} \sum c_{i\alpha} c_{i\beta} c_{i\gamma} f_i^{(0)}$$

$$P_{\alpha\beta} = \partial_\alpha p = \partial_\beta p\, c_s^2 + O(h^2)$$

$$\partial_\beta^{(1)}\partial_\gamma^{(1)} \sum c_{i\alpha} c_{i\beta} c_{i\gamma} \rho w_i\left(1 + \frac{c_{i\sigma} u_\sigma}{c_s^2}\right)$$

$$f_i^{(0)} \approx \rho w_i\left(1 + \frac{c_{i\alpha} u_\alpha}{c_s^2}\right) + O(h^2)$$

Note: $\sum w_i c_{i\alpha} c_{i\beta} c_{i\gamma} c_{i\sigma} = c_s^4(\delta_{\alpha\beta}\delta_{\gamma\sigma} + \delta_{\alpha\gamma}\delta_{\beta\sigma} + \delta_{\alpha\gamma}\delta_{\beta\sigma})$

$$= c_s^2\left(3\partial_\alpha^{(1)}\partial_\alpha^{(1)}(\rho u_1) + 2\partial_1^{(1)}\partial_2^{(1)}(\rho u_2) + \partial_2^{(1)}\partial_2^{(1)}(\rho u_1)\right)$$

$$\to \quad \partial_1^{(1)}\partial_1^{(1)}(\rho u_2) + 2\partial_1^{(1)}\partial_1^{(1)}(\rho u_1) + 3\partial_1^{(1)}\partial_2^{(1)}(\rho u_2) \qquad \alpha = 1,\ \alpha = 2$$

$$= c_s^2\left(\partial_\beta^{(1)}\partial_\beta^{(1)}(\rho u_\alpha) + 2\partial_\alpha^{(1)}\partial_\beta^{(1)}(\rho u_\beta)\right)$$

Note: Mass eqn. $\partial_\beta^{(1)} c_\beta = c_s^2\partial_\beta^{(1)} = c_s^2\partial_\beta^{(1)}(\rho u_\beta + a_\beta)$

$$\partial_t^{(2)}(\rho u_\alpha) - \Delta t\left(\tfrac{1}{2}-\tfrac{1}{\omega}\right)c_s^2\partial_\alpha^{(1)}\partial_\beta^{(1)}(\rho u_\beta) + \Delta t\left(\tfrac{1}{2}-\tfrac{1}{\omega}\right)c_s^2\partial_\beta^{(1)}\partial_\beta^{(1)}(\rho u_\alpha) + 2\left(\partial_\alpha^{(1)}\partial_\beta^{(1)}(\rho u_\beta)\right)$$

$$= \partial_t^{(2)}(\rho u_\alpha) + \Delta t\left(\tfrac{1}{2}-\tfrac{1}{\omega}\right)c_s^2\,\partial_\beta^{(1)}\partial_\beta^{(1)}(\rho u_\alpha) + 3\,\partial_\alpha^{(1)}\underbrace{\partial_\beta^{(1)}(\rho u_\beta)}_{\nabla\cdot\mu_\beta}$$

$$\varepsilon\,\partial_t^{(1)} + \varepsilon^2\partial_t^{(2)} = \partial_t$$

$$\partial_t \rho + \partial_\beta(\rho u_\beta) = 0$$

$$\partial_t(\rho u_\alpha) + \partial_\beta(\rho u_\alpha u_\beta) + \partial_\alpha p = \underbrace{\Delta t\left(\tfrac{1}{\omega}-\tfrac{1}{2}\right)c_s^2\left(\partial_\beta\partial_\beta(\rho u_\alpha) + 2\partial_\alpha(\rho u_\beta)\right)}_{\text{use } \omega \text{ to tune viscosity}}$$

$$\to \partial_\beta\partial_\beta(\rho u_\alpha) \quad u_\alpha \to 0 \quad \nabla^2 u \quad \rho = \text{const}$$

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Numerics of LBM

- Setup of LBM simulation
- Boundary conditions
- Stability

LBM

$$f_i(\underline{x}+c_i, t+1) = f_i(x,t) + \omega\left(f_i^{(eq)}(x,t) - f_i(x,t)\right) \qquad 0<\omega<2$$

$i = 0, \dots, 8$

Two cases:

- time dependent $\left\{ \begin{array}{l} t = 0,1,2 \dots n \\ \longrightarrow \text{treated the same here} \end{array} \right.$
- steady case $\left\{ \begin{array}{l} \longrightarrow t = 0,1,\dots \text{ until } \|u_{n+1} - u_n\| < \varepsilon \end{array} \right.$

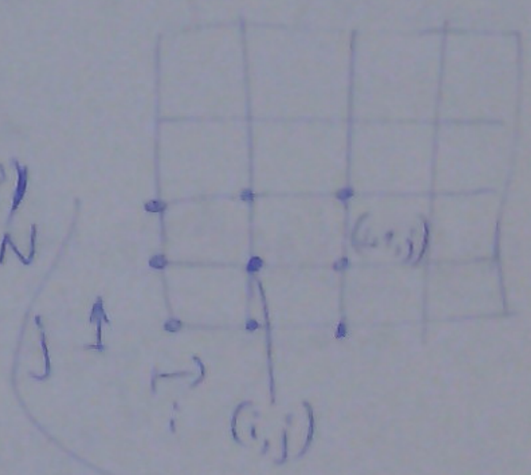
(Alternative $f_i(r+c_i) = f_i(\underline{r}) + \omega\left(f_i^{(eq)}(\underline{r}) - f_i(\underline{r})\right)$)

Recall: Grid topology

Save $f_i^{(eq)}$, f_i as $f(k,i,j)$ $k = 0,\dots,8$; $i,j = 0,\dots,N$

$\rho(i,j)$ etc.

$\underline{u} = (u,v)$ $u(i,j)$ $v(i,j)$



Code outline

initial condition $(\rho_0, \underline{u}_0, \omega)$

$f_i^{(eq)}(\rho_0, u_0) \to f = f^{(eq)}$

do $n = 0, 1, \dots$

$(\rho, \underline{u}) = \text{macroVar}(f)$ $\left\{ \begin{array}{l} \rho = \sum f_i \\ \underline{u} = \frac{1}{\rho}\sum c_i f_i \\ f_i^{(eq)} = \rho w_i\{\dots\} \\ f \leftarrow f + \omega(f^{(eq)} - f) \end{array} \right.$

$f^{(eq)} = \text{computeEq}(\rho, \underline{u})$

apply source terms $f \leftarrow \text{collision}(f, f^{(eq)})$

$f \leftarrow$ apply boundary cond(f)

$f \leftarrow \text{streaming}(f)$ $\quad f_i(r+c_i, t+1) = f_i(r,t)$

end do

Setup of LBM Simulation

Given $\rho^*_{ref}, u^*_{ref}, \nu^*, L$ — dimensional; ν^*: kinematic viscosity

Recall: $f^{(eq)} \propto e^{-\frac{(u-c)^2}{2RT}}$, $(c_s^*)^2$

Pick: Reference Mach no.

eg. $M = 0.01 \Rightarrow (c_s^*) = \frac{u_{ref}}{M}$

$c_0^* = \sqrt{3}\, c_s^*$ (chapter 10)

$\Delta x^* = L/N$

Since $\Delta x^* = c_0^* \Delta t^*$ $\quad \Delta t^* = \frac{\Delta x^*}{c_0^*}$

$t = \frac{t^*}{\Delta t^*}$ $\quad (\Rightarrow \Delta t = 1)$

non-dimensionalize: $c_\alpha = \frac{c_\alpha^*}{c_0^*}$ $\quad \rho = \frac{\rho^*}{\rho^*_{ref}}$

$u_\alpha = \frac{u_\alpha^*}{c_0^*}$ $\quad f = f^*/\rho^*_{ref}$

$c_s = \frac{c_s^*}{c_0^*}$

$$\frac{(f_i^{(eq)})^*}{\rho^*_{ref}} = \frac{\rho^*}{\rho^*_{ref}} w_i \left\{ 1 + \frac{c_i^* \cdot u^*}{c_s^{*2}} + \frac{1}{2}\frac{(c_i^* \cdot u^*)^2}{c_s^{*4}} - \frac{1}{2}\frac{(u^*)^2}{(c_s^*)^2} \right.$$

$$f_i^{(eq)} = \rho w_i \left(1 + \frac{c_i \cdot u}{c_s^2} + \frac{1}{2}\frac{(c_i \cdot u)}{c_s^2} - \frac{1}{2}\frac{u^2}{c_s^2} \right.$$

if $\nu = \frac{\nu^*}{(c_0^*)^2 \Delta t^*}$

$$\frac{\nu}{\Delta t c_s^2} = \frac{1}{\omega} - \frac{1}{2} \rightarrow \omega = \frac{1}{\frac{\nu}{\Delta t c_s^2} + \frac{1}{2}}$$

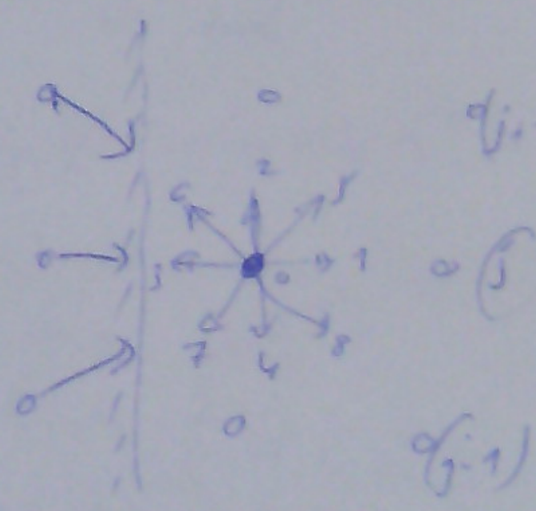
Wall Boundary conditions

assume: after collision step

$f_{8,0,j+1} = f_{6,9,j}$

$f_{1,0,j} = f_{3,9,j}$

$f_{5,0,j} = f_{7,9,j}$



Flux Boundary condition

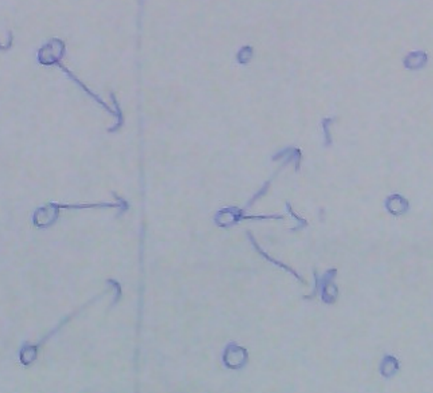
Have (u_0, v_0) @ inflow

want: ρ, f_1, f_5, f_8

Have: moment relations (3 relations)

$\underline{u} = \frac{1}{\rho} \sum c_i f_i$

$\rho = \sum f_i$



extra equation:

$$f_1 - f_1^{eq} = f_3 - f_3^{(eq)} \Rightarrow f_1 = f_3 - (f_3^{eq} - f_1^{eq})$$

$$f_1 = f_3 + \frac{2}{3}\rho u_0$$

$$\rho = \frac{f_0 + f_2 + f_4 + 2(f_3 + f_6 + f_7)}{1 - u_0}$$

$$f_5 = f_7 - \frac{1}{2}(f_2 - f_4) + \frac{1}{6}\rho u_0$$

$$f_8 = f_6 - \frac{1}{2}(f_4 - f_2) + \frac{1}{6}\rho u_0$$

Stability Analysis

Setup: ⊛ Assume infinite Lattice

⊛ $\rho, \underline{u}_0$ be uniform @ $t=0$

i.e $\rho(x,0) = \rho_0$, $\underline{u}(x,0) = \underline{u}_0$ $\Rightarrow f_i^{eq}(x,0) = f_{i,0}^{(eq)} = \text{const}$

⊛ Assume $f_i(x,0)$ is uniform @ $t=0$ (eq $f_i = f_i^{(eq)}$)

i.e $f_i(x,0) = f_{i,0} = \text{const}$ ($\Sigma f_i = \rho_0$ $\Sigma c_i f_i = \rho_0 u_0$

Consider LBM @ $t=0$

$$f_i(x + c_i \Delta t, \Delta t) = f_{i,0} + \omega(f_{i,0}^{(eq)} - f_{i0}) = f_{i,1} \quad (1)$$

(collision is instant)

$$f_{i,1} = (1-\omega) f_{i,0} + \omega f_{i,0}^{(eq)}$$

$$\Sigma f_{i,1} = (1-\omega)\Sigma f_{i,0} + \omega \Sigma f_{i,0}^{(eq)} = \rho \quad (\rho u \text{ similar})$$

Subtract $f_{i,0}^{(eq)}$ from (1)

$$\tilde{f}_{i,1} = f_{i,1} - f_{i,0}^{(eq)} = (1-\omega) f_{i,0} + (\omega - 1) f_{i,0}^{eq}$$

$$= (1-\omega)(f_{i,0} - f_{i,0}^{(eq)})$$

$\tilde{f}_{i,0}$

$$f_{i,2} = (1-\omega) f_{i,1} + \omega f_{i,1}^{(eq)}$$

$f_{i,1}^{(eq)} \rightarrow \rho, u$ are same

Subtract $f_{i,0}^{(eq)}$:

$$\tilde{f}_{i,2} = (1-\omega)\tilde{f}_{i,1} = (1-\omega)^2 \tilde{f}_{i,0}$$

$$\Rightarrow \tilde{f}_{i,k} = (1-\omega)^k \tilde{f}_{i,0}$$

Need $|1-\omega| < 1 \longrightarrow 0 < \omega < 2$

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$H_{01} = \sum_{x \in \mathcal{E}} \left(\sum_i \underbrace{h_i(f_i(x,t))}_{\tilde{h}_i(x,t)} \right)$

~~Introduce Lagrangian~~

H

H. s.t. $\frac{dH}{dt} \leq 0$

$\operatorname{argmin} \{ H^{(g)}(f) : g = \sum f_i^{(0)} ; g_u = \sum c_i f_i^{(0)} \}$

Introduce Lagrangian

$H_1 = \sum_i h_i(f_i) - a(\sum f_i - g) + b(\sum c_i f_i - g_u)$

optimality cond^n

$\frac{\partial H_1}{\partial f_i} = h_i'(f_i) - a - c_i \cdot b \stackrel{!}{=} 0$

$f_i^{(0)} = (h_i')^{-1}(a + b \cdot c_i)$

Show $f_i(t) + w(f_i^{(0)}(t) - f_i(t)) = f(t+1)$

Recall: fundamental theorem of calculus

$\int_0^1 \frac{\partial}{\partial s} g(t+s)\, ds \underset{t+1s=\xi}{=} \int_t^{t+1} g'(\xi)\, d\xi = g(t+1) - g(t)$

Define $f_i(t+s) = f_i(t) + sw(f_i^{(0)}(t) - f_i(t)) \quad 0 \leq s \leq 1$

Let $0 < w < 1$ $\quad \sum f_i(t+s) = g(t+s)$ g_u similar

Then

$\tilde{h}_i(t+1) - \tilde{h}_i(t) = h_i(f_i(t+1)) - h_i(f_i(t))$

$= \int_0^1 \frac{\partial}{\partial s} \{ h_i(f_i(t+s)) \}\, ds$

$= \int_0^1 \frac{\partial}{\partial s} \{ h_i(f_i(t+s)) + a(\sum f_i - g)_{t+s} + b(\sum c_i f_i - g_u)_{t+s} \}\, ds$ (the a-term $= 0$, the b-term $= 0$)

$= \int_0^1 \frac{\partial h_i}{\partial f_i} - a\frac{\partial}{\partial f_i}(\sum f_i - g) - b\frac{\partial}{\partial f_i}(\sum c_i f_i - g_u) \frac{\partial}{\partial s} f_i(t+s)\, ds$

$= + \int_0^1 \underbrace{(h_i' - a - b \cdot c_i)}_{h_i'(f^{(0)})} w(f_i^{(0)} - f_i)|_{t+s}\, ds$ (**)

Note: $f_i(t+s) = f_i(t) + sw(f_i^{(0)} - f_i(t))$ (*)

$f_i(t+s) - f_i(t) = f_i(t) - f_i(t) + sw(f_{i(t)}^{(0)} - f_i(t))$

$= (-1 + sw)(f_i^{(0)}(t) - f_i(t))$

$$\Rightarrow f_i^{(0)} - f_i = \frac{f_i(t+s) - f_i^{(0)}(t)}{s\omega - 1}$$

$$= \frac{f_i^{(0)}(t) - f_i(t+s)}{1 - s\omega}$$

$$(**) = \tilde{h}(f+1) - \tilde{h}(t)$$

$$= \int_0^1 h_i'\big(f(t+s) - h_i'(f^{(0)}(t))\big) \underbrace{\frac{\omega}{1-s\omega}}_{\geq 0} \big(f_i(t) - f_i(t+s)\big)\, ds$$

Δh_i $\quad -\Delta f_i$

h_i convex

$$\frac{\Delta h_i}{\Delta f} \geq 0$$

$$\Delta f \, \Delta h_i' \geq 0$$

$$-\Delta f \, \Delta h_i' \leq 0 \qquad \leq 0$$

$(h_i')^{-1}(x) = a + bx + cx^2$ $\qquad x = \frac{a+b}{c}\cdot c_i$

$a = a(\rho, u) \rightarrow b = b(\rho, u)$

$\sum f_i^{(0)} = \rho \quad \sum f_i^{(0)} c_i = \rho u$

Exam:

Continuum Mechanics

constitutive eqn. relations
eqns. of state

Kinetic theory

- collision models
- Maxwell-Boltzmann → H-theorem
- Boltzmann Eq
- Conservation laws
- Local thermodynamics Equilibrium
  → local maxwellian
  Euler equations
- → BGK eq
- Chapman-Enskog eqn } ⇒ Navier Stokes
  → Diffusion

LGA
Model
Equilibrium → Streaming
Collision
→ H theorem

Shortcomings
(Intermediate models)

LBM

(Derivation)
LB eqn.
moments ($\sum f_i$, $\sum f_i c_i$)
multiscale expansion → coupling with NSE
viscosity
stability
-boundary cond°
- H-Theorem
small compressibility approximation